



\* MINIMIZED COORDINATES FROM CHARMM

\* DATE: 2/25/93

14: 18

CREATED BY USER: nau99

1639

|    |   |     |     |           |           |           |    |   |         |
|----|---|-----|-----|-----------|-----------|-----------|----|---|---------|
| 1  | 1 | ILE | N   | -53.41835 | -52.07964 | 96.86949  | A1 | 1 | 0.00000 |
| 2  | 1 | ILE | HT1 | -54.06550 | -53.37379 | 96.22549  | A1 | 1 | 0.00000 |
| 3  | 1 | ILE | HT2 | -52.48505 | -53.33354 | 96.89426  | A1 | 1 | 0.00000 |
| 4  | 1 | ILE | HT3 | -53.81151 | -52.85195 | 97.84341  | A1 | 1 | 0.00000 |
| 5  | 1 | ILE | CA  | -53.29159 | -51.45945 | 96.52548  | A1 | 1 | 0.00000 |
| 6  | 1 | ILE | CB  | -54.51076 | -51.09296 | 95.64551  | A1 | 1 | 0.00000 |
| 7  | 1 | ILE | CG2 | -55.84867 | -51.39510 | 96.33544  | A1 | 1 | 0.00000 |
| 8  | 1 | ILE | CG1 | -54.43380 | -49.65164 | 95.12978  | A1 | 1 | 0.00000 |
| 9  | 1 | ILE | CD  | -55.55018 | -49.30658 | 94.14124  | A1 | 1 | 0.00000 |
| 10 | 1 | ILE | C   | -53.31306 | -50.79352 | 97.88119  | A1 | 1 | 0.00000 |
| 11 | 1 | ILE | O   | -53.76732 | -51.45486 | 98.80000  | A1 | 1 | 0.00000 |
| 12 | 2 | LYS | N   | -52.70566 | -49.57271 | 97.98462  | A1 | 2 | 0.00000 |
| 13 | 2 | LYS | H   | -52.43149 | -49.07042 | 97.19065  | A1 | 2 | 0.00000 |
| 14 | 2 | LYS | CA  | -52.72856 | -48.82990 | 99.24363  | A1 | 2 | 0.00000 |
| 15 | 2 | LYS | CB  | -51.40674 | -49.22996 | 100.05168 | A1 | 2 | 0.00000 |
| 16 | 2 | LYS | CG  | -51.65942 | -50.46422 | 100.94226 | A1 | 2 | 0.00000 |
| 17 | 2 | LYS | CD  | -50.39491 | -50.76541 | 101.74483 | A1 | 2 | 0.00000 |
| 18 | 2 | LYS | CE  | -50.65567 | -51.67024 | 102.94896 | A1 | 2 | 0.00000 |
| 19 | 2 | LYS | NZ  | -49.48784 | -51.62033 | 103.84066 | A1 | 2 | 0.00000 |
| 20 | 2 | LYS | HZ1 | -49.68891 | -52.15413 | 104.71032 | A1 | 2 | 0.00000 |
| 21 | 2 | LYS | HZ2 | -48.66152 | -52.03086 | 103.36182 | A1 | 2 | 0.00000 |
| 22 | 2 | LYS | HZ3 | -49.20787 | -50.62063 | 104.08530 | A1 | 2 | 0.00000 |
| 23 | 2 | LYS | C   | -52.58080 | -47.37619 | 98.05749  | A1 | 2 | 0.00000 |
| 24 | 2 | LYS | O   | -52.16561 | -47.06993 | 97.74074  | A1 | 2 | 0.00000 |
| 25 | 3 | GLU | N   | -52.93375 | -46.48610 | 99.78817  | A1 | 3 | 0.00000 |
| 26 | 3 | GLU | H   | -53.25920 | -46.74733 | 100.69754 | A1 | 3 | 0.00000 |
| 27 | 3 | GLU | CA  | -52.88416 | -45.05669 | 99.49342  | A1 | 3 | 0.00000 |
| 28 | 3 | GLU | CB  | -54.17633 | -44.67728 | 98.75869  | A1 | 3 | 0.00000 |
| 29 | 3 | GLU | CG  | -54.16941 | -43.30721 | 98.07127  | A1 | 3 | 0.00000 |
| 30 | 3 | GLU | CD  | -55.38365 | -43.14902 | 97.16830  | A1 | 3 | 0.00000 |
| 31 | 3 | GLU | OE1 | -55.40070 | -42.20412 | 96.38367  | A1 | 3 | 0.00000 |
| 32 | 3 | GLU | OE2 | -56.30088 | -43.96983 | 97.23742  | A1 | 3 | 0.00000 |
| 33 | 3 | GLU | C   | -52.73723 | -44.30588 | 100.80334 | A1 | 3 | 0.00000 |
| 34 | 3 | GLU | O   | -53.13310 | -44.80269 | 101.85375 | A1 | 3 | 0.00000 |
| 35 | 4 | GLU | N   | -52.10513 | -43.13147 | 100.72198 | A1 | 4 | 0.00000 |
| 36 | 4 | GLU | H   | -51.89913 | -42.70887 | 99.83885  | A1 | 4 | 0.00000 |
| 37 | 4 | GLU | CA  | -51.71490 | -42.41569 | 101.93532 | A1 | 4 | 0.00000 |
| 38 | 4 | GLU | CB  | -50.23606 | -42.65775 | 102.23912 | A1 | 4 | 0.00000 |
| 39 | 4 | GLU | CG  | -49.88908 | -44.07273 | 102.69972 | A1 | 4 | 0.00000 |
| 40 | 4 | GLU | CD  | -48.39447 | -44.20822 | 102.86978 | A1 | 4 | 0.00000 |
| 41 | 4 | GLU | OE1 | -47.71593 | -43.20739 | 103.12446 | A1 | 4 | 0.00000 |
| 42 | 4 | GLU | OE2 | -47.87485 | -45.31826 | 102.72475 | A1 | 4 | 0.00000 |
| 43 | 4 | GLU | C   | -51.86859 | -40.92476 | 101.75610 | A1 | 4 | 0.00000 |
| 44 | 4 | GLU | O   | -51.85445 | -40.40438 | 100.64776 | A1 | 4 | 0.00000 |
| 45 | 5 | HIS | N   | -51.98758 | -40.25490 | 102.89941 | A1 | 5 | 0.00000 |
| 46 | 5 | HIS | H   | -51.95529 | -40.74179 | 103.77267 | A1 | 5 | 0.00000 |
| 47 | 5 | HIS | CA  | -52.02510 | -38.79739 | 102.88794 | A1 | 5 | 0.00000 |
| 48 | 5 | HIS | CB  | -52.95268 | -38.30654 | 104.00423 | A1 | 5 | 0.00000 |
| 49 | 5 | HIS | CG  | -54.39292 | -38.58657 | 103.64511 | A1 | 5 | 0.00000 |
| 50 | 5 | HIS | ND1 | -55.01336 | -38.04007 | 102.58831 | A1 | 5 | 0.00000 |
| 51 | 5 | HIS | HD1 | -54.63216 | -37.40030 | 101.93314 | A1 | 5 | 0.00000 |
| 52 | 5 | HIS | CD2 | -55.29163 | -39.42491 | 104.31043 | A1 | 5 | 0.00000 |
| 53 | 5 | HIS | NE2 | -56.46563 | -39.37373 | 103.63249 | A1 | 5 | 0.00000 |
| 54 | 5 | HIS | CE1 | -56.29489 | -38.51954 | 102.57197 | A1 | 5 | 0.00000 |
| 55 | 5 | HIS | C   | -50.64149 | -38.20241 | 103.06558 | A1 | 5 | 0.00000 |
| 56 | 5 | HIS | O   | -49.75908 | -38.78174 | 103.68940 | A1 | 5 | 0.00000 |
| 57 | 6 | VAL | N   | -50.46014 | -37.02655 | 102.46317 | A1 | 6 | 0.00000 |
| 58 | 6 | VAL | H   | -51.22869 | -36.59864 | 101.97707 | A1 | 6 | 0.00000 |
| 59 | 6 | VAL | CA  | -49.12695 | -36.41474 | 102.46428 | A1 | 6 | 0.00000 |
| 60 | 6 | VAL | CB  | -48.60121 | -36.23669 | 101.01420 | A1 | 6 | 0.00000 |

FIG. 2

09013077.012698

|     |    |     |      |           |   |           |           |    |    |         |
|-----|----|-----|------|-----------|---|-----------|-----------|----|----|---------|
| 61  | 6  | VAL | CG1  | -47.6     | 2 | -36.30119 | 101.00126 | A1 | 6  | 0.00000 |
| 62  | 6  | VAL | CG2  | -49.10544 |   | -37.46647 | 100.11057 | A1 | 6  | 0.00000 |
| 63  | 6  | VAL | C    | -49.19435 |   | -35.00190 | 103.02675 | A1 | 6  | 0.00000 |
| 64  | 6  | VAL |      | -50.21018 |   | -34.34041 | 102.87457 | A1 | 6  | 0.00000 |
| 65  | 7  | ILE | N    | -48.11527 |   | -34.52120 | 103.65431 | A1 | 7  | 0.00000 |
| 66  | 7  | ILE | H    | -47.35972 |   | -35.13148 | 103.91409 | A1 | 7  | 0.00000 |
| 67  | 7  | ILE | CA   | -48.09506 |   | -33.08697 | 103.98819 | A1 | 7  | 0.00000 |
| 68  | 7  | ILE | CB   | -48.69197 |   | -32.86813 | 105.39701 | A1 | 7  | 0.00000 |
| 69  | 7  | ILE | CG2  | -47.96322 |   | -33.71317 | 106.43001 | A1 | 7  | 0.00000 |
| 70  | 7  | ILE | CG1  | -48.74316 |   | -31.39586 | 105.81727 | A1 | 7  | 0.00000 |
| 71  | 7  | ILE | CD   | -49.28846 |   | -31.20489 | 107.23523 | A1 | 7  | 0.00000 |
| 72  | 7  | ILE | C    | -46.69381 |   | -32.50114 | 103.87753 | A1 | 7  | 0.00000 |
| 73  | 7  | ILE | O    | -45.72315 |   | -33.10109 | 104.32366 | A1 | 7  | 0.00000 |
| 74  | 8  | ILE | N    | -46.61414 |   | -31.32789 | 103.23109 | A1 | 8  | 0.00000 |
| 75  | 8  | ILE | H    | -47.43598 |   | -30.79777 | 103.00074 | A1 | 8  | 0.00000 |
| 76  | 8  | ILE | CA   | -45.31176 |   | -30.85113 | 102.75879 | A1 | 8  | 0.00000 |
| 77  | 8  | ILE | CB   | -45.18096 |   | -31.21426 | 101.24826 | A1 | 8  | 0.00000 |
| 78  | 8  | ILE | CG2  | -46.47692 |   | -30.98133 | 100.47371 | A1 | 8  | 0.00000 |
| 79  | 8  | ILE | CG1  | -44.01581 |   | -30.53590 | 100.51961 | A1 | 8  | 0.00000 |
| 80  | 8  | ILE | CD   | -42.65515 |   | -30.85297 | 101.12422 | A1 | 8  | 0.00000 |
| 81  | 8  | ILE | C    | -45.00402 |   | -29.37643 | 103.03239 | A1 | 8  | 0.00000 |
| 82  | 8  | ILE | O    | -45.69216 |   | -28.43922 | 102.63903 | A1 | 8  | 0.00000 |
| 83  | 9  | GLN | N    | -43.86371 |   | -29.19466 | 103.70229 | A1 | 9  | 0.00000 |
| 84  | 9  | GLN | H    | -43.33777 |   | -29.97409 | 104.05676 | A1 | 9  | 0.00000 |
| 85  | 9  | GLN | CA   | -43.27910 |   | -27.85712 | 103.71549 | A1 | 9  | 0.00000 |
| 86  | 9  | GLN | CB   | -42.97213 |   | -27.43231 | 105.14730 | A1 | 9  | 0.00000 |
| 87  | 9  | GLN | CG   | -44.24353 |   | -27.13894 | 105.94550 | A1 | 9  | 0.00000 |
| 88  | 9  | GLN | CD   | -43.92932 |   | -26.69043 | 107.36359 | A1 | 9  | 0.00000 |
| 89  | 9  | GLN | OE1  | -44.59992 |   | -27.05224 | 108.31811 | A1 | 9  | 0.00000 |
| 90  | 9  | GLN | NE2  | -42.89278 |   | -25.86874 | 107.50418 | A1 | 9  | 0.00000 |
| 91  | 9  | GLN | HE21 | -42.31986 |   | -25.58069 | 106.73881 | A1 | 9  | 0.00000 |
| 92  | 9  | GLN | HE22 | -42.66204 |   | -25.53260 | 108.41526 | A1 | 9  | 0.00000 |
| 93  | 9  | GLN | C    | -42.00840 |   | -27.79728 | 102.89330 | A1 | 9  | 0.00000 |
| 94  | 9  | GLN | O    | -41.07030 |   | -28.56703 | 103.06902 | A1 | 9  | 0.00000 |
| 95  | 10 | ALA | N    | -42.01720 |   | -26.84230 | 101.96835 | A1 | 10 | 0.00000 |
| 96  | 10 | ALA | H    | -42.80016 |   | -26.24022 | 101.81084 | A1 | 10 | 0.00000 |
| 97  | 10 | ALA | CA   | -40.33464 |   | -26.60034 | 101.15833 | A1 | 10 | 0.00000 |
| 98  | 10 | ALA | CB   | -41.09424 |   | -26.95993 | 99.69281  | A1 | 10 | 0.00000 |
| 99  | 10 | ALA | C    | -40.41733 |   | -25.14834 | 101.25674 | A1 | 10 | 0.00000 |
| 100 | 10 | ALA | O    | -41.21138 |   | -24.24680 | 101.50542 | A1 | 10 | 0.00000 |
| 101 | 11 | GLU | N    | -39.11637 |   | -24.95043 | 101.08226 | A1 | 11 | 0.00000 |
| 102 | 11 | GLU | H    | -38.51800 |   | -25.72332 | 100.86462 | A1 | 11 | 0.00000 |
| 103 | 11 | GLU | CA   | -38.56697 |   | -23.61077 | 101.26935 | A1 | 11 | 0.00000 |
| 104 | 11 | GLU | CB   | -37.61570 |   | -23.62729 | 102.46404 | A1 | 11 | 0.00000 |
| 105 | 11 | GLU | CG   | -38.29740 |   | -24.15021 | 103.73032 | A1 | 11 | 0.00000 |
| 106 | 11 | GLU | CD   | -37.31724 |   | -24.35236 | 104.86668 | A1 | 11 | 0.00000 |
| 107 | 11 | GLU | OE1  | -37.72498 |   | -24.91514 | 105.87939 | A1 | 11 | 0.00000 |
| 108 | 11 | GLU | OE2  | -36.15746 |   | -23.95826 | 104.74301 | A1 | 11 | 0.00000 |
| 109 | 11 | GLU | C    | -37.79619 |   | -23.17941 | 100.04756 | A1 | 11 | 0.00000 |
| 110 | 11 | GLU | O    | -37.17390 |   | -23.59314 | 99.37097  | A1 | 11 | 0.00000 |
| 111 | 12 | PHE | N    | -37.86688 |   | -21.67280 | 99.78525  | A1 | 12 | 0.00000 |
| 112 | 12 | PHE | H    | -38.38856 |   | -21.25141 | 100.37827 | A1 | 12 | 0.00000 |
| 113 | 12 | PHE | CA   | -37.20863 |   | -21.33691 | 98.59813  | A1 | 12 | 0.00000 |
| 114 | 12 | PHE | CB   | -38.26225 |   | -21.06791 | 97.51950  | A1 | 12 | 0.00000 |
| 115 | 12 | PHE | CG   | -37.93682 |   | -21.86124 | 96.27668  | A1 | 12 | 0.00000 |
| 116 | 12 | PHE | CD1  | -38.35291 |   | -23.20899 | 96.17465  | A1 | 12 | 0.00000 |
| 117 | 12 | PHE | CD2  | -37.21678 |   | -21.25353 | 95.22261  | A1 | 12 | 0.00000 |
| 118 | 12 | PHE | CE1  | -38.04712 |   | -23.95258 | 95.01356  | A1 | 12 | 0.00000 |
| 119 | 12 | PHE | CE2  | -36.91098 |   | -21.99741 | 94.06122  | A1 | 12 | 0.00000 |
| 120 | 12 | PHE | CZ   | -37.32685 |   | -23.34453 | 93.96022  | A1 | 12 | 0.00000 |
| 121 | 12 | PHE | C    | -36.45949 |   | -20.05659 | 98.90209  | A1 | 12 | 0.00000 |
| 122 | 12 | PHE | O    | -37.00216 |   | -18.95008 | 98.93077  | A1 | 12 | 0.00000 |
| 123 | 13 | TYR | N    | -35.16677 |   | -20.22034 | 99.15293  | A1 | 13 | 0.00000 |
| 124 | 13 | TYR | H    | -34.71888 |   | -21.10886 | 99.03348  | A1 | 13 | 0.00000 |

FIG. 3

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|     |    |     |      |           |           |           |    |    |         |
|-----|----|-----|------|-----------|-----------|-----------|----|----|---------|
| 125 | 13 | TYR | CA   | -34.44    | -19.02891 | 99.57908  | A1 | 13 | 7.00000 |
| 126 | 13 | TYR | CB   | -33.741   | -19.31637 | 100.90471 | A1 | 13 | 0.00000 |
| 127 | 13 | TYR | CG   | -33.63229 | -18.04844 | 101.71489 | A1 | 13 | 0.00000 |
| 128 | 13 | TYR | CD1  | -34.79192 | -17.52707 | 102.32828 | A1 | 13 | 0.00000 |
| 129 | 13 | TYR | CE1  | -34.69736 | -16.35710 | 103.10470 | A1 | 13 | 0.00000 |
| 130 | 13 | TYR | CD2  | -32.38328 | -17.40687 | 101.86606 | A1 | 13 | 0.00000 |
| 131 | 13 | TYR | CE2  | -32.29405 | -16.23332 | 102.64552 | A1 | 13 | 0.00000 |
| 132 | 13 | TYR | CZ   | -33.45188 | -15.71594 | 103.26657 | A1 | 13 | 0.00000 |
| 133 | 13 | TYR | OH   | -33.37191 | -14.58930 | 104.06109 | A1 | 13 | 0.00000 |
| 134 | 13 | TYR | HH   | -33.47343 | -14.89238 | 104.98360 | A1 | 13 | 0.00000 |
| 135 | 13 | TYR | C    | -33.46702 | -18.52544 | 98.54525  | A1 | 13 | 0.00000 |
| 136 | 13 | TYR | O    | -32.59456 | -19.23915 | 98.06786  | A1 | 13 | 0.00000 |
| 137 | 14 | LEU | N    | -33.65240 | -17.25550 | 98.19697  | A1 | 14 | 0.00000 |
| 138 | 14 | LEU | H    | -34.33538 | -16.68306 | 98.64807  | A1 | 14 | 0.00000 |
| 139 | 14 | LEU | CA   | -32.81168 | -16.70428 | 97.14258  | A1 | 14 | 0.00000 |
| 140 | 14 | LEU | CB   | -33.70274 | -16.21044 | 96.00105  | A1 | 14 | 0.00000 |
| 141 | 14 | LEU | CG   | -33.98219 | -17.29674 | 94.96260  | A1 | 14 | 0.00000 |
| 142 | 14 | LEU | CD1  | -35.16863 | -16.92524 | 94.07539  | A1 | 14 | 0.00000 |
| 143 | 14 | LEU | CD2  | -32.72461 | -17.54798 | 94.13078  | A1 | 14 | 0.00000 |
| 144 | 14 | LEU | C    | -31.93377 | -15.56813 | 97.60481  | A1 | 14 | 0.00000 |
| 145 | 14 | LEU | O    | -32.31049 | -14.71998 | 98.40126  | A1 | 14 | 0.00000 |
| 146 | 15 | ASN | N    | -30.73908 | -15.58168 | 97.02166  | A1 | 15 | 0.00000 |
| 147 | 15 | ASN | H    | -30.47955 | -16.38705 | 96.48149  | A1 | 15 | 0.00000 |
| 148 | 15 | ASN | CA   | -29.88530 | -14.39297 | 97.02352  | A1 | 15 | 0.00000 |
| 149 | 15 | ASN | CB   | -28.47094 | -14.93729 | 97.29287  | A1 | 15 | 0.00000 |
| 150 | 15 | ASN | CG   | -27.86774 | -14.18957 | 98.46652  | A1 | 15 | 0.00000 |
| 151 | 15 | ASN | OD1  | -28.47231 | -13.98878 | 99.50693  | A1 | 15 | 0.00000 |
| 152 | 15 | ASN | ND2  | -26.63329 | -13.74712 | 98.26721  | A1 | 15 | 0.00000 |
| 153 | 15 | ASN | HD21 | -26.12722 | -13.93409 | 97.42633  | A1 | 15 | 0.00000 |
| 154 | 15 | ASN | HD22 | -26.21377 | -13.18778 | 98.98020  | A1 | 15 | 0.00000 |
| 155 | 15 | ASN | C    | -30.09328 | -13.70870 | 95.65633  | A1 | 15 | 0.00000 |
| 156 | 15 | ASN | O    | -30.96066 | -14.17929 | 94.92357  | A1 | 15 | 0.00000 |
| 157 | 16 | PRO | N    | -29.35358 | -12.64312 | 95.25454  | A1 | 16 | 0.00000 |
| 158 | 16 | PRO | CD   | -29.47390 | -12.14147 | 93.88390  | A1 | 16 | 0.00000 |
| 159 | 16 | PRO | CA   | -28.34388 | -11.89943 | 96.02164  | A1 | 16 | 0.00000 |
| 160 | 16 | PRO | CB   | -27.47317 | -11.32145 | 94.90180  | A1 | 16 | 0.00000 |
| 161 | 16 | PRO | CG   | -28.40713 | -11.06430 | 93.72211  | A1 | 16 | 0.00000 |
| 162 | 16 | PRO | C    | -28.67201 | -10.84560 | 96.98393  | A1 | 16 | 0.00000 |
| 163 | 16 | PRO | O    | -28.49727 | -10.81095 | 98.14625  | A1 | 16 | 0.00000 |
| 164 | 17 | ASP | N    | -29.73099 | -9.96981  | 96.45979  | A1 | 17 | 0.00000 |
| 165 | 17 | ASP | H    | -30.06531 | -10.06794 | 95.52595  | A1 | 17 | 0.00000 |
| 166 | 17 | ASP | CA   | -30.07647 | -8.75629  | 97.18869  | A1 | 17 | 0.00000 |
| 167 | 17 | ASP | CB   | -30.80318 | -7.83976  | 96.20071  | A1 | 17 | 0.00000 |
| 168 | 17 | ASP | CG   | -30.22601 | -6.44601  | 96.27578  | A1 | 17 | 0.00000 |
| 169 | 17 | ASP | OD1  | -29.42577 | -6.10216  | 95.40955  | A1 | 17 | 0.00000 |
| 170 | 17 | ASP | OD2  | -30.58500 | -5.71147  | 97.19272  | A1 | 17 | 0.00000 |
| 171 | 17 | ASP | C    | -30.91226 | -8.96778  | 98.44177  | A1 | 17 | 0.00000 |
| 172 | 17 | ASP | O    | -30.52677 | -8.65960  | 99.56331  | A1 | 17 | 0.00000 |
| 173 | 18 | GLN | N    | -32.11780 | -9.49744  | 90.20428  | A1 | 18 | 0.00000 |
| 174 | 18 | GLN | H    | -32.36542 | -9.81984  | 97.29256  | A1 | 18 | 0.00000 |
| 175 | 18 | GLN | CA   | -33.10696 | -9.57864  | 99.27949  | A1 | 18 | 0.00000 |
| 176 | 18 | GLN | CB   | -34.05728 | -8.37464  | 99.14180  | A1 | 18 | 0.00000 |
| 177 | 18 | GLN | CG   | -33.36307 | -7.07517  | 99.58476  | A1 | 18 | 0.00000 |
| 178 | 18 | GLN | CD   | -33.97880 | -5.85158  | 98.94046  | A1 | 18 | 0.00000 |
| 179 | 18 | GLN | OE1  | -35.13776 | -5.50918  | 99.12725  | A1 | 18 | 0.00000 |
| 180 | 18 | GLN | NE2  | -33.14378 | -5.16835  | 98.16624  | A1 | 18 | 0.00000 |
| 181 | 18 | GLN | HE21 | -32.19859 | -5.47544  | 97.99847  | A1 | 18 | 0.00000 |
| 182 | 18 | GLN | HE22 | -33.43475 | -4.32502  | 97.72302  | A1 | 18 | 0.00000 |
| 183 | 18 | GLN | C    | -33.83924 | -10.91598 | 99.26964  | A1 | 18 | 0.00000 |
| 184 | 18 | GLN | O    | -33.74750 | -11.68763 | 98.32391  | A1 | 18 | 0.00000 |
| 185 | 19 | SER | N    | -34.51482 | -11.16924 | 100.39831 | A1 | 19 | 0.00000 |
| 186 | 19 | SER | H    | -34.63228 | -10.43017 | 101.06649 | A1 | 19 | 0.00000 |
| 187 | 19 | SER | CA   | -34.94474 | -12.50816 | 100.83625 | A1 | 19 | 0.00000 |
| 188 | 19 | SER | CB   | -35.43672 | -12.36114 | 102.28173 | A1 | 19 | 0.00000 |

FIG. 4

09013077.012698

|     |    |     |     |           |   |           |           |    |    |         |
|-----|----|-----|-----|-----------|---|-----------|-----------|----|----|---------|
| 189 | 19 | SER | OG  | -34.3     | 1 | -11.87727 | 103.10841 | A1 | 19 | 0.00000 |
| 190 | 19 | SER | HG  | -33.85    | 4 | -12.63499 | 103.40254 | A1 | 19 | 0.00000 |
| 191 | 19 | SER | C   | -35.97640 |   | -13.29776 | 100.02197 | A1 | 19 | 0.00000 |
| 192 | 19 | SER | O   | -36.49518 |   | -12.86400 | 99.00144  | A1 | 19 | 0.00000 |
| 193 | 20 | GLY | N   | -36.24917 |   | -14.51787 | 100.53004 | A1 | 20 | 0.00000 |
| 194 | 20 | GLY | H   | -35.87834 |   | -14.79673 | 101.41380 | A1 | 20 | 0.00000 |
| 195 | 20 | GLY | CA  | -37.08223 |   | -15.47533 | 99.79192  | A1 | 20 | 0.00000 |
| 196 | 20 | GLY | C   | -38.39897 |   | -15.89747 | 100.44590 | A1 | 20 | 0.00000 |
| 197 | 20 | GLY | O   | -39.10838 |   | -15.10421 | 101.05171 | A1 | 20 | 0.00000 |
| 198 | 21 | GLU | N   | -38.72023 |   | -17.18722 | 100.25477 | A1 | 21 | 0.00000 |
| 199 | 21 | GLU | H   | -38.03254 |   | -17.84573 | 99.94375  | A1 | 21 | 0.00000 |
| 200 | 21 | GLU | CA  | -40.11538 |   | -17.64629 | 100.27114 | A1 | 21 | 0.00000 |
| 201 | 21 | GLU | CB  | -40.54163 |   | -17.64420 | 98.79559  | A1 | 21 | 0.00000 |
| 202 | 21 | GLU | CG  | -42.00974 |   | -17.90322 | 98.44054  | A1 | 21 | 0.00000 |
| 203 | 21 | GLU | CD  | -42.16555 |   | -17.98331 | 96.93169  | A1 | 21 | 0.00000 |
| 204 | 21 | GLU | OE1 | -43.22010 |   | -17.59671 | 96.43390  | A1 | 21 | 0.00000 |
| 205 | 21 | GLU | OE2 | -41.23758 |   | -18.43207 | 96.25678  | A1 | 21 | 0.00000 |
| 206 | 21 | GLU | C   | -40.28326 |   | -19.04137 | 100.89226 | A1 | 21 | 0.00000 |
| 207 | 21 | GLU | O   | -39.32286 |   | -19.78361 | 101.07437 | A1 | 21 | 0.00000 |
| 208 | 22 | PHE | N   | -41.54286 |   | -19.38051 | 101.22645 | A1 | 22 | 0.00000 |
| 209 | 22 | PHE | H   | -42.30204 |   | -18.76344 | 101.01655 | A1 | 22 | 0.00000 |
| 210 | 22 | PHE | CA  | -41.84777 |   | -20.63223 | 101.93252 | A1 | 22 | 0.00000 |
| 211 | 22 | PHE | CB  | -41.76716 |   | -20.31207 | 103.43794 | A1 | 22 | 0.00000 |
| 212 | 22 | PHE | CG  | -41.45246 |   | -21.48591 | 104.34752 | A1 | 22 | 0.00000 |
| 213 | 22 | PHE | CD1 | -40.59481 |   | -21.25886 | 105.44915 | A1 | 22 | 0.00000 |
| 214 | 22 | PHE | CD2 | -42.01384 |   | -22.76966 | 104.14562 | A1 | 22 | 0.00000 |
| 215 | 22 | PHE | CE1 | -40.30109 |   | -22.30643 | 106.34948 | A1 | 22 | 0.00000 |
| 216 | 22 | PHE | CE2 | -41.72224 |   | -23.81970 | 105.04232 | A1 | 22 | 0.00000 |
| 217 | 22 | PHE | CZ  | -40.86722 |   | -23.58408 | 106.14281 | A1 | 22 | 0.00000 |
| 218 | 22 | PHE | C   | -43.25845 |   | -21.11908 | 101.58028 | A1 | 22 | 0.00000 |
| 219 | 22 | PHE | O   | -44.19436 |   | -20.32985 | 101.55111 | A1 | 22 | 0.00000 |
| 220 | 23 | MET | N   | -43.39639 |   | -22.43138 | 101.32298 | A1 | 23 | 0.00000 |
| 221 | 23 | MET | H   | -42.59132 |   | -23.03279 | 101.30500 | A1 | 23 | 0.00000 |
| 222 | 23 | MET | CA  | -44.70480 |   | -23.04357 | 101.02967 | A1 | 23 | 0.00000 |
| 223 | 23 | MET | CB  | -45.08326 |   | -22.73266 | 99.57140  | A1 | 23 | 0.00000 |
| 224 | 23 | MET | CG  | -46.39952 |   | -23.35273 | 99.09264  | A1 | 23 | 0.00000 |
| 225 | 23 | MET | SD  | -46.67153 |   | -23.10231 | 97.33272  | A1 | 23 | 0.00000 |
| 226 | 23 | MET | CE  | -47.47592 |   | -24.67640 | 96.98955  | A1 | 23 | 0.00000 |
| 227 | 23 | MET | C   | -44.60710 |   | -24.56281 | 101.21411 | A1 | 23 | 0.00000 |
| 228 | 23 | MET | O   | -43.70841 |   | -25.13566 | 100.62115 | A1 | 23 | 0.00000 |
| 229 | 24 | PHE | N   | -45.43241 |   | -25.30285 | 101.99622 | A1 | 24 | 0.00000 |
| 230 | 24 | PHE | H   | -45.17063 |   | -26.26850 | 102.03772 | A1 | 24 | 0.00000 |
| 231 | 24 | PHE | CA  | -46.72021 |   | -25.11140 | 102.69060 | A1 | 24 | 0.00000 |
| 232 | 24 | PHE | CB  | -47.06193 |   | -23.70552 | 103.21139 | A1 | 24 | 0.00000 |
| 233 | 24 | PHE | CG  | -46.27878 |   | -23.27691 | 104.43188 | A1 | 24 | 0.00000 |
| 234 | 24 | PHE | CD1 | -46.28203 |   | -24.06677 | 105.60532 | A1 | 24 | 0.00000 |
| 235 | 24 | PHE | CD2 | -45.58233 |   | -22.04683 | 104.40480 | A1 | 24 | 0.00000 |
| 236 | 24 | PHE | CE1 | -45.58915 |   | -23.62279 | 106.75356 | A1 | 24 | 0.00000 |
| 237 | 24 | PHE | CE2 | -46.89083 |   | -21.60100 | 105.55271 | A1 | 24 | 0.00000 |
| 238 | 24 | PHE | CZ  | -46.89594 |   | -22.39162 | 106.72434 | A1 | 24 | 0.00000 |
| 239 | 24 | PHE | C   | -47.88569 |   | -25.61775 | 101.85776 | A1 | 24 | 0.00000 |
| 240 | 24 | PHE | O   | -48.73152 |   | -24.07778 | 101.36424 | A1 | 24 | 0.00000 |
| 241 | 25 | ASP | N   | -47.89055 |   | -26.94593 | 101.74049 | A1 | 25 | 0.00000 |
| 242 | 25 | ASP | H   | -47.22437 |   | -27.52403 | 102.20704 | A1 | 25 | 0.00000 |
| 243 | 25 | ASP | CA  | -48.86501 |   | -27.64762 | 100.90165 | A1 | 25 | 0.00000 |
| 244 | 25 | ASP | CB  | -48.21052 |   | -27.81535 | 99.52046  | A1 | 25 | 0.00000 |
| 245 | 25 | ASP | CG  | -49.19634 |   | -28.30012 | 98.47932  | A1 | 25 | 0.00000 |
| 246 | 25 | ASP | OD1 | -49.75750 |   | -27.46672 | 97.77589  | A1 | 25 | 0.00000 |
| 247 | 25 | ASP | OD2 | -49.39656 |   | -29.50745 | 98.36197  | A1 | 25 | 0.00000 |
| 248 | 25 | ASP | C   | -49.18430 |   | -28.98699 | 101.56183 | A1 | 25 | 0.00000 |
| 249 | 25 | ASP | O   | -48.57317 |   | -29.35714 | 102.56241 | A1 | 25 | 0.00000 |
| 250 | 26 | PHE | N   | -50.15619 |   | -29.70261 | 101.00377 | A1 | 26 | 0.00000 |
| 251 | 26 | PHE | H   | -50.60050 |   | -29.38662 | 100.15349 | A1 | 26 | 0.00000 |
| 252 | 26 | PHE | CA  | -50.56030 |   | -30.88701 | 101.54898 | A1 | 26 | 0.00000 |

FIG. 5

09013077 012598

|     |    |     |     |           |           |           |    |    |         |
|-----|----|-----|-----|-----------|-----------|-----------|----|----|---------|
| 253 | 26 | PHE | CB  | -51.78    | -30.83090 | 102.82009 | A1 | 26 | 0.00000 |
| 254 | 26 | PHE | CG  | -52.60356 | -29.92038 | 102.57724 | A1 | 26 | 0.00000 |
| 255 | 26 | PHE | CD1 | -52.50398 | -28.55674 | 102.91777 | A1 | 26 | 0.00000 |
| 256 | 26 | PHE | CD2 | -53.70380 | -30.42265 | 101.99011 | A1 | 26 | 0.00000 |
| 257 | 26 | PHE | CE1 | -53.58477 | -27.68701 | 102.66706 | A1 | 26 | 0.00000 |
| 258 | 26 | PHE | CE2 | -54.86474 | -29.55076 | 101.74257 | A1 | 26 | 0.00000 |
| 259 | 26 | PHE | CZ  | -54.76149 | -28.18547 | 102.07912 | A1 | 26 | 0.00000 |
| 260 | 26 | PHE | C   | -51.29340 | -31.82500 | 100.51070 | A1 | 26 | 0.00000 |
| 261 | 26 | PHE | O   | -51.63257 | -31.38211 | 99.42184  | A1 | 26 | 0.00000 |
| 262 | 27 | ASP | N   | -51.50640 | -33.00225 | 100.89199 | A1 | 27 | 0.00000 |
| 263 | 27 | ASP | H   | -51.30608 | -33.34660 | 101.83544 | A1 | 27 | 0.00000 |
| 264 | 27 | ASP | CA  | -52.05815 | -34.11623 | 100.01741 | A1 | 27 | 0.00000 |
| 265 | 27 | ASP | CB  | -53.56271 | -34.25359 | 100.24733 | A1 | 27 | 0.00000 |
| 266 | 27 | ASP | CG  | -53.82295 | -35.66101 | 100.73899 | A1 | 27 | 0.00000 |
| 267 | 27 | ASP | OD1 | -52.95640 | -36.23164 | 101.40272 | A1 | 27 | 0.00000 |
| 268 | 27 | ASP | OD2 | -54.89062 | -36.19966 | 100.47314 | A1 | 27 | 0.00000 |
| 269 | 27 | ASP | C   | -51.70102 | -34.05698 | 98.54820  | A1 | 27 | 0.00000 |
| 270 | 27 | ASP | O   | -52.51335 | -34.10386 | 97.63254  | A1 | 27 | 0.00000 |
| 271 | 28 | GLY | N   | -50.39045 | -33.92246 | 98.35075  | A1 | 28 | 0.00000 |
| 272 | 28 | GLY | H   | -49.78144 | -33.80079 | 99.13160  | A1 | 28 | 0.00000 |
| 273 | 28 | GLY | CA  | -49.88845 | -33.86633 | 96.98221  | A1 | 28 | 0.00000 |
| 274 | 28 | GLY | C   | -50.00090 | -32.51821 | 96.28701  | A1 | 28 | 0.00000 |
| 275 | 28 | GLY | O   | -49.04304 | -32.03342 | 95.69731  | A1 | 28 | 0.00000 |
| 276 | 29 | ASP | N   | -51.21573 | -31.96145 | 96.33541  | A1 | 29 | 0.00000 |
| 277 | 29 | ASP | H   | -51.93955 | -32.39453 | 96.87595  | A1 | 29 | 0.00000 |
| 278 | 29 | ASP | CA  | -51.52130 | -30.85124 | 95.43198  | A1 | 29 | 0.00000 |
| 279 | 29 | ASP | CB  | -52.38232 | -31.44665 | 94.30287  | A1 | 29 | 0.00000 |
| 280 | 29 | ASP | CG  | -52.46245 | -30.54960 | 93.07581  | A1 | 29 | 0.00000 |
| 281 | 29 | ASP | OD1 | -51.43429 | -30.32445 | 92.44162  | A1 | 29 | 0.00000 |
| 282 | 29 | ASP | OD2 | -53.56233 | -30.10545 | 92.75048  | A1 | 29 | 0.00000 |
| 283 | 29 | ASP | C   | -52.21461 | -29.64631 | 96.07233  | A1 | 29 | 0.00000 |
| 284 | 29 | ASP | O   | -52.39419 | -28.59407 | 95.46732  | A1 | 29 | 0.00000 |
| 285 | 30 | GLU | N   | -52.65130 | -29.81701 | 97.32405  | A1 | 30 | 0.00000 |
| 286 | 30 | GLU | H   | -52.34793 | -30.57647 | 97.90251  | A1 | 30 | 0.00000 |
| 287 | 30 | GLU | CA  | -53.43516 | -28.70871 | 97.86160  | A1 | 30 | 0.00000 |
| 288 | 30 | GLU | CB  | -54.71008 | -29.18152 | 98.54724  | A1 | 30 | 0.00000 |
| 289 | 30 | GLU | CG  | -55.04100 | -29.71506 | 97.67444  | A1 | 30 | 0.00000 |
| 290 | 30 | GLU | CD  | -57.13279 | -29.50058 | 98.43828  | A1 | 30 | 0.00000 |
| 291 | 30 | GLU | OE1 | -57.79466 | -30.47326 | 98.78969  | A1 | 30 | 0.00000 |
| 292 | 30 | GLU | OE2 | -57.48939 | -28.34297 | 98.66447  | A1 | 30 | 0.00000 |
| 293 | 30 | GLU | C   | -52.69655 | -27.80995 | 98.82987  | A1 | 30 | 0.00000 |
| 294 | 30 | GLU | O   | -52.13191 | -28.20198 | 99.84476  | A1 | 30 | 0.00000 |
| 295 | 31 | ILE | N   | -52.76110 | -26.53268 | 98.46810  | A1 | 31 | 0.00000 |
| 296 | 31 | ILE | H   | -53.28532 | -26.29454 | 97.65353  | A1 | 31 | 0.00000 |
| 297 | 31 | ILE | CA  | -51.98442 | -25.52556 | 99.18511  | A1 | 31 | 0.00000 |
| 298 | 31 | ILE | CB  | -51.81933 | -24.32331 | 98.23317  | A1 | 31 | 0.00000 |
| 299 | 31 | ILE | CG2 | -53.16329 | -23.65625 | 97.91607  | A1 | 31 | 0.00000 |
| 300 | 31 | ILE | CG1 | -50.75168 | -23.33810 | 98.71478  | A1 | 31 | 0.00000 |
| 301 | 31 | ILE | CD  | -50.41981 | -22.27940 | 97.66271  | A1 | 31 | 0.00000 |
| 302 | 31 | ILE | C   | -52.51316 | -25.12446 | 100.56211 | A1 | 31 | 0.00000 |
| 303 | 31 | ILE | O   | -53.70233 | -24.97567 | 100.82175 | A1 | 31 | 0.00000 |
| 304 | 32 | PHE | N   | -51.54696 | -24.95576 | 101.46562 | A1 | 32 | 0.00000 |
| 305 | 32 | PHE | H   | -50.59061 | -25.06998 | 101.18020 | A1 | 32 | 0.00000 |
| 306 | 32 | PHE | CA  | -51.85606 | -24.57978 | 102.84494 | A1 | 32 | 0.00000 |
| 307 | 32 | PHE | CB  | -50.76201 | -25.18703 | 103.73391 | A1 | 32 | 0.00000 |
| 308 | 32 | PHE | CG  | -51.19588 | -26.22218 | 104.74893 | A1 | 32 | 0.00000 |
| 309 | 32 | PHE | CD1 | -50.23927 | -27.18148 | 105.15120 | A1 | 32 | 0.00000 |
| 310 | 32 | PHE | CD2 | -52.49149 | -26.22907 | 105.32111 | A1 | 32 | 0.00000 |
| 311 | 32 | PHE | CE1 | -50.57386 | -28.14516 | 106.12524 | A1 | 32 | 0.00000 |
| 312 | 32 | PHE | CE2 | -52.82688 | -27.19600 | 106.29575 | A1 | 32 | 0.00000 |
| 313 | 32 | PHE | CZ  | -51.86606 | -26.15152 | 106.69566 | A1 | 32 | 0.00000 |
| 314 | 32 | PHE | C   | -51.84397 | -23.87181 | 103.07985 | A1 | 32 | 0.00000 |
| 315 | 32 | PHE | O   | -52.76581 | -22.44086 | 103.62205 | A1 | 32 | 0.00000 |
| 316 | 33 | HIS | N   | -50.69098 | -22.54451 | 102.70813 | A1 | 33 | 0.00000 |

FIG. 6

09013077.012698

|     |    |     |     |           |           |           |    |    |         |
|-----|----|-----|-----|-----------|-----------|-----------|----|----|---------|
| 317 | 33 | HIS | H   | -50.04    | -22.98834 | 102.10706 | A1 | 33 | 0.00000 |
| 318 | 33 | HIS | CA  | -50.22    | -21.21727 | 103.23242 | A1 | 33 | 0.00000 |
| 319 | 33 | HIS | CB  | -49.65908 | -21.51540 | 104.63303 | A1 | 33 | 0.00000 |
| 320 | 33 | HIS | CG  | -49.22984 | -20.32142 | 105.45366 | A1 | 33 | 0.00000 |
| 321 | 33 | HIS | ND1 | -48.02826 | -19.72793 | 105.37205 | A1 | 33 | 0.00000 |
| 322 | 33 | HIS | HD1 | -47.28999 | -19.92757 | 104.75923 | A1 | 33 | 0.00000 |
| 323 | 33 | HIS | CD2 | -49.97214 | -19.68828 | 106.45019 | A1 | 33 | 0.00000 |
| 324 | 33 | HIS | NE2 | -49.20118 | -18.70682 | 106.97086 | A1 | 33 | 0.00000 |
| 325 | 33 | HIS | CE1 | -48.00110 | -18.72654 | 106.30763 | A1 | 33 | 0.00000 |
| 326 | 33 | HIS | C   | -49.11511 | -20.78472 | 102.29629 | A1 | 33 | 0.00000 |
| 327 | 33 | HIS | O   | -48.59725 | -21.61206 | 101.55845 | A1 | 33 | 0.00000 |
| 328 | 34 | VAL | N   | -48.74537 | -19.50449 | 102.33695 | A1 | 34 | 0.00000 |
| 329 | 34 | VAL | H   | -49.19429 | -18.80802 | 102.90183 | A1 | 34 | 0.00000 |
| 330 | 34 | VAL | CA  | -47.51776 | -19.11490 | 101.64269 | A1 | 34 | 0.00000 |
| 331 | 34 | VAL | CB  | -47.81303 | -18.42567 | 100.28392 | A1 | 34 | 0.00000 |
| 332 | 34 | VAL | CG1 | -46.56686 | -18.41158 | 99.39158  | A1 | 34 | 0.00000 |
| 333 | 34 | VAL | CG2 | -48.95871 | -19.06363 | 99.49806  | A1 | 34 | 0.00000 |
| 334 | 34 | VAL | C   | -46.79652 | -18.14692 | 102.56509 | A1 | 34 | 0.00000 |
| 335 | 34 | VAL | O   | -47.41849 | -17.54298 | 103.42874 | A1 | 34 | 0.00000 |
| 336 | 35 | ASP | N   | -45.47963 | -18.03426 | 102.37666 | A1 | 35 | 0.00000 |
| 337 | 35 | ASP | H   | -45.03039 | -18.68906 | 101.76710 | A1 | 35 | 0.00000 |
| 338 | 35 | ASP | CA  | -44.68799 | -16.93300 | 102.93355 | A1 | 35 | 0.00000 |
| 339 | 35 | ASP | CB  | -44.74876 | -15.73492 | 101.94639 | A1 | 35 | 0.00000 |
| 340 | 35 | ASP | CG  | -46.11850 | -15.06364 | 101.88569 | A1 | 35 | 0.00000 |
| 341 | 35 | ASP | OD1 | -46.85196 | -15.31279 | 100.93528 | A1 | 35 | 0.00000 |
| 342 | 35 | ASP | CD2 | -46.43780 | -14.28565 | 102.78747 | A1 | 35 | 0.00000 |
| 343 | 35 | ASP | C   | -44.90949 | -16.57120 | 104.41152 | A1 | 35 | 0.00000 |
| 344 | 35 | ASP | O   | -45.03304 | -17.43137 | 105.27733 | A1 | 35 | 0.00000 |
| 345 | 36 | MET | N   | -44.91212 | -15.26386 | 104.68945 | A1 | 36 | 0.00000 |
| 346 | 36 | MET | H   | -44.97503 | -14.56792 | 103.95356 | A1 | 36 | 0.00000 |
| 347 | 36 | MET | CA  | -45.05621 | -14.74244 | 106.04065 | A1 | 36 | 0.00000 |
| 348 | 36 | MET | CB  | -44.58443 | -13.28473 | 106.01845 | A1 | 36 | 0.00000 |
| 349 | 36 | MET | CG  | -43.15122 | -13.10955 | 105.50403 | A1 | 36 | 0.00000 |
| 350 | 36 | MET | SD  | -42.96722 | -11.71848 | 104.37016 | A1 | 36 | 0.00000 |
| 351 | 36 | MET | CE  | -43.60204 | -10.40582 | 105.42531 | A1 | 36 | 0.00000 |
| 352 | 36 | MET | C   | -46.49207 | -14.77022 | 106.53712 | A1 | 36 | 0.00000 |
| 353 | 36 | MET | O   | -46.75425 | -14.73983 | 107.73458 | A1 | 36 | 0.00000 |
| 354 | 37 | ALA | N   | -47.43476 | -14.70996 | 105.58618 | A1 | 37 | 0.00000 |
| 355 | 37 | ALA | H   | -47.21869 | -14.67225 | 104.60519 | A1 | 37 | 0.00000 |
| 356 | 37 | ALA | CA  | -48.80100 | -14.57493 | 106.05297 | A1 | 37 | 0.00000 |
| 357 | 37 | ALA | CB  | -49.30059 | -13.19637 | 105.61316 | A1 | 37 | 0.00000 |
| 358 | 37 | ALA | C   | -49.83252 | -15.61256 | 105.65673 | A1 | 37 | 0.00000 |
| 359 | 37 | ALA | O   | -49.85254 | -16.18787 | 104.57639 | A1 | 37 | 0.00000 |
| 360 | 38 | LYS | N   | -50.76933 | -15.79391 | 106.59397 | A1 | 38 | 0.00000 |
| 361 | 38 | LYS | H   | -50.65212 | -15.37866 | 107.49351 | A1 | 38 | 0.00000 |
| 362 | 38 | LYS | CA  | -52.00981 | -16.48765 | 106.23832 | A1 | 38 | 0.00000 |
| 363 | 38 | LYS | CB  | -52.90628 | -16.55867 | 107.48306 | A1 | 38 | 0.00000 |
| 364 | 38 | LYS | CG  | -52.41585 | -17.40517 | 108.60236 | A1 | 38 | 0.00000 |
| 365 | 38 | LYS | CD  | -53.40991 | -18.62084 | 108.86903 | A1 | 38 | 0.00000 |
| 366 | 38 | LYS | CE  | -53.42547 | -19.66155 | 107.75111 | A1 | 38 | 0.00000 |
| 367 | 38 | LYS | NZ  | -54.78503 | -20.17861 | 107.56038 | A1 | 38 | 0.00000 |
| 368 | 38 | LYS | HZ1 | -54.79226 | -20.92377 | 106.83759 | A1 | 38 | 0.00000 |
| 369 | 38 | LYS | HZ2 | -55.17879 | -20.59510 | 108.44046 | A1 | 38 | 0.00000 |
| 370 | 38 | LYS | HZ3 | -55.42747 | -19.41621 | 107.27224 | A1 | 38 | 0.00000 |
| 371 | 38 | LYS | C   | -52.74081 | -15.73437 | 105.12989 | A1 | 38 | 0.00000 |
| 372 | 38 | LYS | O   | -52.72521 | -14.51209 | 105.10297 | A1 | 38 | 0.00000 |
| 373 | 39 | LYS | N   | -53.35457 | -16.44351 | 104.17702 | A1 | 39 | 0.00000 |
| 374 | 39 | LYS | H   | -53.59774 | -15.96113 | 103.33578 | A1 | 39 | 0.00000 |
| 375 | 39 | LYS | CA  | -53.67982 | -17.86931 | 104.22041 | A1 | 39 | 0.00000 |
| 376 | 39 | LYS | CB  | -55.18971 | -18.00306 | 104.55246 | A1 | 39 | 0.00000 |
| 377 | 39 | LYS | CG  | -56.24681 | -17.84030 | 103.42417 | A1 | 39 | 0.00000 |
| 378 | 39 | LYS | CD  | -56.27039 | -16.52550 | 102.62130 | A1 | 39 | 0.00000 |
| 379 | 39 | LYS | CE  | -56.64532 | -16.49161 | 101.13213 | A1 | 39 | 0.00000 |
| 380 | 39 | LYS | NZ  | -55.66137 | -17.54082 | 100.43822 | A1 | 39 | 0.00000 |

FIG. 7

0501307 013698

|     |    |     |      |           |    |           |           |    |    |         |
|-----|----|-----|------|-----------|----|-----------|-----------|----|----|---------|
| 381 | 39 | LYS | H21  | -55.1     | 45 | -18.54581 | 100.36313 | A1 | 39 | 0.00000 |
| 382 | 39 | LYS | H22  | -55.1     | 53 | -17.26725 | 99.46103  | A1 | 39 | 0.00000 |
| 383 | 39 | LYS | H23  | -54.72486 |    | -17.51921 | 100.90690 | A1 | 39 | 0.00000 |
| 384 | 39 | LYS | C    | -53.44423 |    | -18.44283 | 102.84433 | A1 | 39 | 0.00000 |
| 385 | 39 | LYS | O    | -53.43351 |    | -17.67518 | 101.88936 | A1 | 39 | 0.00000 |
| 386 | 40 | GLU | N    | -53.41332 |    | -19.77420 | 102.71885 | A1 | 40 | 0.00000 |
| 387 | 40 | GLU | H    | -53.16154 |    | -20.43691 | 103.42697 | A1 | 40 | 0.00000 |
| 388 | 40 | GLU | CA   | -54.08892 |    | -20.14645 | 101.48663 | A1 | 40 | 0.00000 |
| 389 | 40 | GLU | CB   | -53.22132 |    | -20.84643 | 100.44056 | A1 | 40 | 0.00000 |
| 390 | 40 | GLU | CG   | -52.68203 |    | -19.82757 | 99.41114  | A1 | 40 | 0.00000 |
| 391 | 40 | GLU | CD   | -53.78227 |    | -10.90107 | 98.89631  | A1 | 40 | 0.00000 |
| 392 | 40 | GLU | OE1  | -53.60681 |    | -17.68372 | 98.89245  | A1 | 40 | 0.00000 |
| 393 | 40 | GLU | OE2  | -54.88246 |    | -19.35560 | 98.59153  | A1 | 40 | 0.00000 |
| 394 | 40 | GLU | C    | -55.46625 |    | -20.74566 | 101.61501 | A1 | 40 | 0.00000 |
| 395 | 40 | GLU | O    | -56.42031 |    | -20.18304 | 101.08479 | A1 | 40 | 0.00000 |
| 396 | 41 | THR | N    | -55.56321 |    | -21.84976 | 102.35754 | A1 | 41 | 0.00000 |
| 397 | 41 | THR | H    | -54.77319 |    | -22.20472 | 102.86321 | A1 | 41 | 0.00000 |
| 398 | 41 | THR | CA   | -56.84476 |    | -22.55464 | 102.30963 | A1 | 41 | 0.00000 |
| 399 | 41 | THR | CB   | -56.55011 |    | -24.05030 | 102.16109 | A1 | 41 | 0.00000 |
| 400 | 41 | THR | OG1  | -57.73042 |    | -24.75407 | 101.74066 | A1 | 41 | 0.00000 |
| 401 | 41 | THR | HG1  | -57.47835 |    | -25.59614 | 101.33840 | A1 | 41 | 0.00000 |
| 402 | 41 | THR | CG2  | -55.95304 |    | -24.67173 | 103.43152 | A1 | 41 | 0.00000 |
| 403 | 41 | THR | C    | -57.85722 |    | -22.26510 | 103.42344 | A1 | 41 | 0.00000 |
| 404 | 41 | THR | O    | -57.54877 |    | -21.93546 | 104.56718 | A1 | 41 | 0.00000 |
| 405 | 42 | VAL | N    | -59.12316 |    | -22.41525 | 103.00455 | A1 | 42 | 0.00000 |
| 406 | 42 | VAL | H    | -59.25687 |    | -22.81422 | 102.09633 | A1 | 42 | 0.00000 |
| 407 | 42 | VAL | CA   | -60.29134 |    | -22.03291 | 103.80812 | A1 | 42 | 0.00000 |
| 408 | 42 | VAL | CB   | -61.57611 |    | -22.26646 | 102.98525 | A1 | 42 | 0.00000 |
| 409 | 42 | VAL | CG1  | -62.83989 |    | -21.83994 | 103.74041 | A1 | 42 | 0.00000 |
| 410 | 42 | VAL | CG2  | -61.49852 |    | -21.55078 | 101.63610 | A1 | 42 | 0.00000 |
| 411 | 42 | VAL | C    | -60.39368 |    | -22.75550 | 105.14170 | A1 | 42 | 0.00000 |
| 412 | 42 | VAL | O    | -60.54018 |    | -22.16641 | 106.20404 | A1 | 42 | 0.00000 |
| 413 | 43 | TRP | N    | -60.26652 |    | -24.07997 | 105.07466 | A1 | 43 | 0.00000 |
| 414 | 43 | TRP | H    | -60.09540 |    | -24.53437 | 104.20145 | A1 | 43 | 0.00000 |
| 415 | 43 | TRP | CA   | -60.35178 |    | -24.82113 | 106.34002 | A1 | 43 | 0.00000 |
| 416 | 43 | TRP | CB   | -60.91225 |    | -26.25321 | 106.17013 | A1 | 43 | 0.00000 |
| 417 | 43 | TRP | CG   | -60.96314 |    | -26.72686 | 104.73262 | A1 | 43 | 0.00000 |
| 418 | 43 | TRP | CD2  | -59.88712 |    | -27.12198 | 103.92127 | A1 | 43 | 0.00000 |
| 419 | 43 | TRP | CE2  | -60.47947 |    | -27.49629 | 102.60102 | A1 | 43 | 0.00000 |
| 420 | 43 | TRP | CE3  | -58.50029 |    | -27.24274 | 104.12574 | A1 | 43 | 0.00000 |
| 421 | 43 | TRP | CD1  | -62.11826 |    | -26.86040 | 103.93459 | A1 | 43 | 0.00000 |
| 422 | 43 | TRP | HE1  | -61.84174 |    | -27.31306 | 102.67766 | A1 | 43 | 0.00000 |
| 423 | 43 | TRP | HE1  | -62.50030 |    | -27.49046 | 101.97106 | A1 | 43 | 0.00000 |
| 424 | 43 | TRP | CZ2  | -59.62565 |    | -27.96652 | 101.58525 | A1 | 43 | 0.00000 |
| 425 | 43 | TRP | CZ3  | -57.69263 |    | -27.72260 | 103.07694 | A1 | 43 | 0.00000 |
| 426 | 43 | TRP | CH2  | -58.24204 |    | -28.07937 | 101.82597 | A1 | 43 | 0.00000 |
| 427 | 43 | TRP | C    | -59.07150 |    | -24.84373 | 107.16564 | A1 | 43 | 0.00000 |
| 428 | 43 | TRP | O    | -58.85050 |    | -25.68073 | 100.02836 | A1 | 43 | 0.00000 |
| 429 | 44 | ARG | N    | -58.22471 |    | -23.84563 | 106.89519 | A1 | 44 | 0.00000 |
| 430 | 44 | ARG | H    | -58.31398 |    | -23.27977 | 106.07364 | A1 | 44 | 0.00000 |
| 431 | 44 | ARG | CA   | -57.22046 |    | -23.49560 | 107.89144 | A1 | 44 | 0.00000 |
| 432 | 44 | ARG | CB   | -55.83244 |    | -23.69727 | 107.26013 | A1 | 44 | 0.00000 |
| 433 | 44 | ARG | CG   | -54.63741 |    | -23.63473 | 108.22026 | A1 | 44 | 0.00000 |
| 434 | 44 | ARG | CD   | -53.30915 |    | -23.64273 | 107.47006 | A1 | 44 | 0.00000 |
| 435 | 44 | ARG | HE   | -52.10625 |    | -23.26000 | 108.32672 | A1 | 44 | 0.00000 |
| 436 | 44 | ARG | HE   | -52.36221 |    | -22.91543 | 109.25139 | A1 | 44 | 0.00000 |
| 437 | 44 | ARG | CZ   | -50.93149 |    | -23.33650 | 107.86475 | A1 | 44 | 0.00000 |
| 438 | 44 | ARG | NH1  | -49.92358 |    | -22.86519 | 108.56844 | A1 | 44 | 0.00000 |
| 439 | 44 | ARG | NH11 | -48.98076 |    | -22.84912 | 108.24673 | A1 | 44 | 0.00000 |
| 440 | 44 | ARG | NH12 | -50.05182 |    | -22.52238 | 109.51721 | A1 | 44 | 0.00000 |
| 441 | 44 | ARG | NH2  | -50.67215 |    | -23.89024 | 106.69352 | A1 | 44 | 0.00000 |
| 442 | 44 | ARG | NH21 | -49.73581 |    | -23.96008 | 106.35139 | A1 | 44 | 0.00000 |
| 443 | 44 | ARG | NH22 | -51.41769 |    | -24.25918 | 106.14195 | A1 | 44 | 0.00000 |
| 444 | 44 | ARG | C    | -57.42751 |    | -22.85857 | 108.38029 | A1 | 44 | 0.00000 |

FIG. 8

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|     |    |     |      |           |   |           |           |    |    |         |
|-----|----|-----|------|-----------|---|-----------|-----------|----|----|---------|
| 445 | 44 | ARG | O    | -56.5     | 4 | -21.39201 | 108.88943 | A1 | 44 | 0.00000 |
| 446 | 45 | LEU | N    | -58.65270 |   | -21.55686 | 108.18548 | A1 | 45 | 0.00000 |
| 447 | 45 | LEU | H    | -59.36846 |   | -22.06382 | 107.69729 | A1 | 45 | 0.00000 |
| 448 | 45 | LEU | CA   | -58.94679 |   | -20.21897 | 108.70611 | A1 | 45 | 0.00000 |
| 449 | 45 | LEU | CB   | -59.87267 |   | -19.46515 | 107.74942 | A1 | 45 | 0.00000 |
| 450 | 45 | LEU | CG   | -59.15056 |   | -18.96990 | 106.49579 | A1 | 45 | 0.00000 |
| 451 | 45 | LEU | CD1  | -60.14534 |   | -18.41906 | 105.47407 | A1 | 45 | 0.00000 |
| 452 | 45 | LEU | CD2  | -58.10431 |   | -17.92289 | 106.87944 | A1 | 45 | 0.00000 |
| 453 | 45 | LEU | C    | -59.55818 |   | -20.20104 | 110.09168 | A1 | 45 | 0.00000 |
| 454 | 45 | LEU | O    | -59.53362 |   | -19.19926 | 110.79199 | A1 | 45 | 0.00000 |
| 455 | 46 | GLU | N    | -60.08917 |   | -21.36024 | 110.48954 | A1 | 46 | 0.00000 |
| 456 | 46 | GLU | H    | -60.14047 |   | -22.14708 | 109.87631 | A1 | 46 | 0.00000 |
| 457 | 46 | GLU | CA   | -60.58379 |   | -21.47317 | 111.86481 | A1 | 46 | 0.00000 |
| 458 | 46 | GLU | CB   | -61.47817 |   | -22.71518 | 111.95437 | A1 | 46 | 0.00000 |
| 459 | 46 | GLU | CG   | -60.80881 |   | -24.02305 | 111.51772 | A1 | 46 | 0.00000 |
| 460 | 46 | GLU | CD   | -61.85264 |   | -25.11830 | 111.46594 | A1 | 46 | 0.00000 |
| 461 | 46 | GLU | OE1  | -62.26867 |   | -25.47222 | 110.36424 | A1 | 46 | 0.00000 |
| 462 | 46 | GLU | OE2  | -62.24894 |   | -25.60616 | 112.52280 | A1 | 46 | 0.00000 |
| 463 | 46 | GLU | C    | -59.48698 |   | -21.49323 | 112.92683 | A1 | 46 | 0.00000 |
| 464 | 46 | GLU | O    | -59.60959 |   | -21.22226 | 114.10493 | A1 | 46 | 0.00000 |
| 465 | 47 | GLU | N    | -58.27880 |   | -21.79310 | 112.44220 | A1 | 47 | 0.00000 |
| 466 | 47 | GLU | H    | -58.18142 |   | -22.06659 | 111.48920 | A1 | 47 | 0.00000 |
| 467 | 47 | GLU | CA   | -57.08155 |   | -21.73864 | 113.27698 | A1 | 47 | 0.00000 |
| 468 | 47 | GLU | CB   | -55.89121 |   | -22.09481 | 112.39059 | A1 | 47 | 0.00000 |
| 469 | 47 | GLU | CG   | -55.95036 |   | -23.50661 | 111.78977 | A1 | 47 | 0.00000 |
| 470 | 47 | GLU | CD   | -55.55418 |   | -24.59648 | 112.78701 | A1 | 47 | 0.00000 |
| 471 | 47 | GLU | OE1  | -55.48886 |   | -25.74409 | 112.37878 | A1 | 47 | 0.00000 |
| 472 | 47 | GLU | OE2  | -55.29749 |   | -24.27876 | 113.95212 | A1 | 47 | 0.00000 |
| 473 | 47 | GLU | C    | -56.83827 |   | -20.38151 | 113.91510 | A1 | 47 | 0.00000 |
| 474 | 47 | GLU | O    | -56.67000 |   | -19.35742 | 113.26194 | A1 | 47 | 0.00000 |
| 475 | 48 | PHE | N    | -56.83807 |   | -20.40716 | 115.24713 | A1 | 48 | 0.00000 |
| 476 | 48 | PHE | H    | -56.92233 |   | -21.28123 | 115.72305 | A1 | 48 | 0.00000 |
| 477 | 48 | PHE | CA   | -56.75617 |   | -19.13647 | 115.96362 | A1 | 48 | 0.00000 |
| 478 | 48 | PHE | CB   | -57.20231 |   | -19.34982 | 117.41420 | A1 | 48 | 0.00000 |
| 479 | 48 | PHE | CG   | -58.41657 |   | -18.49841 | 117.70829 | A1 | 48 | 0.00000 |
| 480 | 48 | PHE | CD1  | -59.71122 |   | -19.00320 | 117.44215 | A1 | 48 | 0.00000 |
| 481 | 48 | PHE | CD2  | -58.25459 |   | -17.19966 | 118.24455 | A1 | 48 | 0.00000 |
| 482 | 48 | PHE | CE1  | -60.04630 |   | -18.20670 | 117.71246 | A1 | 48 | 0.00000 |
| 483 | 48 | PHE | CE2  | -59.38540 |   | -16.40286 | 118.51469 | A1 | 48 | 0.00000 |
| 484 | 48 | PHE | CZ   | -60.66202 |   | -16.90878 | 118.24779 | A1 | 48 | 0.00000 |
| 485 | 48 | PHE | C    | -55.39240 |   | -18.46628 | 115.93777 | A1 | 48 | 0.00000 |
| 486 | 48 | PHE | O    | -54.35117 |   | -19.07618 | 115.72587 | A1 | 48 | 0.00000 |
| 487 | 49 | GLY | N    | -55.43214 |   | -17.15361 | 116.19781 | A1 | 49 | 0.00000 |
| 488 | 49 | GLY | H    | -56.32069 |   | -16.72101 | 116.34575 | A1 | 49 | 0.00000 |
| 489 | 49 | GLY | CA   | -54.23420 |   | -16.30520 | 116.13162 | A1 | 49 | 0.00000 |
| 490 | 49 | GLY | C    | -52.92695 |   | -16.86464 | 116.68056 | A1 | 49 | 0.00000 |
| 491 | 49 | GLY | O    | -51.85815 |   | -16.69886 | 116.10714 | A1 | 49 | 0.00000 |
| 492 | 50 | ARG | N    | -53.03915 |   | -17.56211 | 117.81779 | A1 | 50 | 0.00000 |
| 493 | 50 | ARG | H    | -53.93660 |   | -17.67284 | 118.24069 | A1 | 50 | 0.00000 |
| 494 | 50 | ARG | CA   | -51.84656 |   | -18.16800 | 118.42224 | A1 | 50 | 0.00000 |
| 495 | 50 | ARG | CB   | -52.27437 |   | -18.92760 | 119.68340 | A1 | 50 | 0.00000 |
| 496 | 50 | ARG | CG   | -51.10260 |   | -19.32736 | 120.56254 | A1 | 50 | 0.00000 |
| 497 | 50 | ARG | CD   | -51.53002 |   | -20.14774 | 121.80047 | A1 | 50 | 0.00000 |
| 498 | 50 | ARG | NE   | -50.37432 |   | -20.44943 | 122.64580 | A1 | 50 | 0.00000 |
| 499 | 50 | ARG | HE   | -49.69865 |   | -19.71957 | 122.75767 | A1 | 50 | 0.00000 |
| 500 | 50 | ARG | CZ   | -50.24449 |   | -21.63184 | 123.26571 | A1 | 50 | 0.00000 |
| 501 | 50 | ARG | NH1  | -49.18578 |   | -21.04466 | 124.04503 | A1 | 50 | 0.00000 |
| 502 | 50 | ARG | NH11 | -49.05579 |   | -22.71179 | 124.52612 | A1 | 50 | 0.00000 |
| 503 | 50 | ARG | NH12 | -48.49360 |   | -21.13233 | 124.16453 | A1 | 50 | 0.00000 |
| 504 | 50 | ARG | NH2  | -51.15926 |   | -22.58629 | 123.10823 | A1 | 50 | 0.00000 |
| 505 | 50 | ARG | NH21 | -51.08073 |   | -23.47414 | 123.56513 | A1 | 50 | 0.00000 |
| 506 | 50 | ARG | NH22 | -51.95092 |   | -22.42795 | 122.51852 | A1 | 50 | 0.00000 |
| 507 | 50 | ARG | C    | -51.06703 |   | -19.09581 | 117.49074 | A1 | 50 | 0.00000 |
| 508 | 50 | ARG | O    | -49.84240 |   | -19.09133 | 117.41826 | A1 | 50 | 0.00000 |

FIG. 9

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|     |    |     |      |           |           |           |    |    |         |
|-----|----|-----|------|-----------|-----------|-----------|----|----|---------|
| 509 | 51 | PHE | N    | -51.84    | -19.87778 | 116.73839 | A1 | 51 | 0.00000 |
| 510 | 51 | PHE | H    | -52.84564 | -19.76657 | 116.76797 | A1 | 51 | 0.00000 |
| 511 | 51 | PHE | CA   | -51.29477 | -20.78796 | 115.73402 | A1 | 51 | 0.00000 |
| 512 | 51 | PHE | CB   | -52.51672 | -21.52503 | 115.15449 | A1 | 51 | 0.00000 |
| 513 | 51 | PHE | CG   | -52.25099 | -22.49194 | 114.02359 | A1 | 51 | 0.00000 |
| 514 | 51 | PHE | CD1  | -51.87888 | -23.82851 | 114.29503 | A1 | 51 | 0.00000 |
| 515 | 51 | PHE | CD2  | -52.45788 | -22.06484 | 112.69289 | A1 | 51 | 0.00000 |
| 516 | 51 | PHE | CE1  | -51.72483 | -24.74421 | 113.22969 | A1 | 51 | 0.00000 |
| 517 | 51 | PHE | CE2  | -52.30778 | -22.98082 | 111.63059 | A1 | 51 | 0.00000 |
| 518 | 51 | PHE | CZ   | -51.94314 | -24.31860 | 111.90000 | A1 | 51 | 0.00000 |
| 519 | 51 | PHE | C    | -50.50268 | -20.00696 | 114.69371 | A1 | 51 | 0.00000 |
| 520 | 51 | PHE | O    | -49.31281 | -20.20801 | 114.47961 | A1 | 51 | 0.00000 |
| 521 | 52 | ALA | N    | -51.20469 | -19.03212 | 114.10202 | A1 | 52 | 0.00000 |
| 522 | 52 | ALA | H    | -52.16823 | -18.89764 | 114.33870 | A1 | 52 | 0.00000 |
| 523 | 52 | ALA | CA   | -50.54896 | -18.16486 | 113.11957 | A1 | 52 | 0.00000 |
| 524 | 52 | ALA | CB   | -51.52058 | -17.09216 | 112.62511 | A1 | 52 | 0.00000 |
| 525 | 52 | ALA | C    | -49.28257 | -17.48933 | 113.62687 | A1 | 52 | 0.00000 |
| 526 | 52 | ALA | O    | -48.27008 | -17.39834 | 112.94510 | A1 | 52 | 0.00000 |
| 527 | 53 | SER | N    | -49.35763 | -17.04955 | 114.88764 | A1 | 53 | 0.00000 |
| 528 | 53 | SER | H    | -50.22411 | -17.11498 | 115.38567 | A1 | 53 | 0.00000 |
| 529 | 53 | SER | CA   | -48.18100 | -16.47055 | 115.53815 | A1 | 53 | 0.00000 |
| 530 | 53 | SER | CB   | -48.58146 | -16.02158 | 116.95383 | A1 | 53 | 0.00000 |
| 531 | 53 | SER | OG   | -47.59593 | -15.15541 | 117.52845 | A1 | 53 | 0.00000 |
| 532 | 53 | SER | HG   | -47.05158 | -14.90357 | 118.42105 | A1 | 53 | 0.00000 |
| 533 | 53 | SER | C    | -46.99433 | -17.42737 | 115.57426 | A1 | 53 | 0.00000 |
| 534 | 53 | SER | O    | -45.89463 | -17.11790 | 115.12568 | A1 | 53 | 0.00000 |
| 535 | 54 | PHE | N    | -47.26082 | -18.64220 | 116.08200 | A1 | 54 | 0.00000 |
| 536 | 54 | PHE | H    | -40.18040 | -10.87361 | 116.41568 | A1 | 54 | 0.00000 |
| 537 | 54 | PHE | CA   | -46.18727 | -19.64350 | 116.09999 | A1 | 54 | 0.00000 |
| 538 | 54 | PHE | CB   | -46.69548 | -20.99079 | 116.63413 | A1 | 54 | 0.00000 |
| 539 | 54 | PHE | CG   | -46.90625 | -20.99411 | 118.13255 | A1 | 54 | 0.00000 |
| 540 | 54 | PHE | CD1  | -48.11656 | -21.50316 | 118.65539 | A1 | 54 | 0.00000 |
| 541 | 54 | PHE | CD2  | -45.89246 | -20.53119 | 119.00621 | A1 | 54 | 0.00000 |
| 542 | 54 | PHE | CE1  | -48.31310 | -21.55376 | 120.05266 | A1 | 54 | 0.00000 |
| 543 | 54 | PHE | CE2  | -46.08593 | -20.57973 | 120.40382 | A1 | 54 | 0.00000 |
| 544 | 54 | PHE | CZ   | -47.30008 | -21.09192 | 120.92307 | A1 | 54 | 0.00000 |
| 545 | 54 | PHE | C    | -45.57270 | -19.90650 | 114.73758 | A1 | 54 | 0.00000 |
| 546 | 54 | PHE | O    | -44.36030 | -19.93109 | 114.55246 | A1 | 54 | 0.00000 |
| 547 | 55 | GLU | N    | -46.46681 | -20.08976 | 113.76558 | A1 | 55 | 0.00000 |
| 548 | 55 | GLU | H    | -47.45338 | -20.04226 | 113.95516 | A1 | 55 | 0.00000 |
| 549 | 55 | GLU | CA   | -45.97322 | -20.41545 | 112.42886 | A1 | 55 | 0.00000 |
| 550 | 55 | GLU | CB   | -47.14512 | -20.81915 | 111.54876 | A1 | 55 | 0.00000 |
| 551 | 55 | GLU | CG   | -47.92567 | -21.96126 | 112.19274 | A1 | 55 | 0.00000 |
| 552 | 55 | GLU | CD   | -49.04456 | -22.36202 | 111.27677 | A1 | 55 | 0.00000 |
| 553 | 55 | GLU | OE1  | -49.15553 | -23.53977 | 110.96047 | A1 | 55 | 0.00000 |
| 554 | 55 | GLU | OE2  | -49.80524 | -21.50984 | 110.81474 | A1 | 55 | 0.00000 |
| 555 | 55 | GLU | C    | -45.19354 | -19.30188 | 111.76318 | A1 | 55 | 0.00000 |
| 556 | 55 | GLU | O    | -44.12678 | -19.50387 | 111.19343 | A1 | 55 | 0.00000 |
| 557 | 56 | ALA | N    | -45.73650 | -18.08673 | 111.89532 | A1 | 56 | 0.00000 |
| 558 | 56 | ALA | H    | -46.62336 | -17.96765 | 112.34890 | A1 | 56 | 0.00000 |
| 559 | 56 | ALA | CA   | -45.00414 | -16.92733 | 111.38640 | A1 | 56 | 0.00000 |
| 560 | 56 | ALA | CB   | -45.80074 | -15.63871 | 111.59969 | A1 | 56 | 0.00000 |
| 561 | 56 | ALA | C    | -43.63772 | -16.77849 | 112.02791 | A1 | 56 | 0.00000 |
| 562 | 56 | ALA | O    | -42.62065 | -16.60634 | 111.36878 | A1 | 56 | 0.00000 |
| 563 | 57 | GLN | N    | -43.63088 | -16.91454 | 113.35929 | A1 | 57 | 0.00000 |
| 564 | 57 | GLN | H    | -44.46826 | -17.03983 | 113.86832 | A1 | 57 | 0.00000 |
| 565 | 57 | GLN | CA   | -42.35063 | -16.88200 | 114.06847 | A1 | 57 | 0.00000 |
| 566 | 57 | GLN | CB   | -42.61967 | -17.03049 | 115.56930 | A1 | 57 | 0.00000 |
| 567 | 57 | GLN | CG   | -41.40659 | -16.75355 | 116.45895 | A1 | 57 | 0.00000 |
| 568 | 57 | GLN | CD   | -41.80070 | -16.94529 | 117.90800 | A1 | 57 | 0.00000 |
| 569 | 57 | GLN | OE1  | -42.29879 | -16.06206 | 118.58910 | A1 | 57 | 0.00000 |
| 570 | 57 | GLN | OE2  | -41.55425 | -10.16011 | 116.38366 | A1 | 57 | 0.00000 |
| 571 | 57 | GLN | HE21 | -41.14709 | -18.27176 | 117.81428 | A1 | 57 | 0.00000 |
| 572 | 57 | GLN | HE22 | -41.78115 | -18.35728 | 119.33313 | A1 | 57 | 0.00000 |

FIG. 10

09013077.012698

|     |    |     |      |           |           |           |    |    |         |
|-----|----|-----|------|-----------|-----------|-----------|----|----|---------|
| 573 | 57 | GLN | C    | -41.13    | -17.94055 | 113.59025 | A1 | 57 | 0.00000 |
| 574 | 57 | GLN | O    | -40.18571 | -17.68051 | 113.34773 | A1 | 57 | 0.00000 |
| 575 | 58 | GLY | N    | -41.88825 | -19.15742 | 113.41319 | A1 | 58 | 0.00000 |
| 576 | 58 | GLY | H    | -42.84771 | -19.33514 | 113.64847 | A1 | 58 | 0.00000 |
| 577 | 58 | GLY | CA   | -41.05379 | -20.23393 | 112.87374 | A1 | 58 | 0.00000 |
| 578 | 58 | GLY | C    | -40.45534 | -19.92701 | 111.50957 | A1 | 58 | 0.00000 |
| 579 | 58 | GLY | O    | -39.25324 | -20.01021 | 111.27849 | A1 | 58 | 0.00000 |
| 580 | 59 | ALA | N    | -41.34654 | -19.52227 | 110.60018 | A1 | 59 | 0.00000 |
| 581 | 59 | ALA | H    | -42.32072 | -19.46762 | 110.83485 | A1 | 59 | 0.00000 |
| 582 | 59 | ALA | CA   | -40.88666 | -19.14537 | 109.26181 | A1 | 59 | 0.00000 |
| 583 | 59 | ALA | CB   | -42.07124 | -18.74086 | 108.30101 | A1 | 59 | 0.00000 |
| 584 | 59 | ALA | C    | -39.86090 | -18.02257 | 109.26073 | A1 | 59 | 0.00000 |
| 585 | 59 | ALA | O    | -38.85187 | -18.04905 | 108.56603 | A1 | 59 | 0.00000 |
| 586 | 60 | LEU | N    | -40.12979 | -17.02925 | 110.11113 | A1 | 60 | 0.00000 |
| 587 | 60 | LEU | H    | -40.96678 | -17.03715 | 110.66448 | A1 | 60 | 0.00000 |
| 588 | 60 | LEU | CA   | -39.17026 | -15.93079 | 110.21454 | A1 | 60 | 0.00000 |
| 589 | 60 | LEU | CB   | -39.62974 | -14.72108 | 110.88234 | A1 | 60 | 0.00000 |
| 590 | 60 | LEU | CG   | -41.00342 | -14.16448 | 110.06267 | A1 | 60 | 0.00000 |
| 591 | 60 | LEU | CD1  | -41.72077 | -13.05637 | 110.83175 | A1 | 60 | 0.00000 |
| 592 | 60 | LEU | CD2  | -40.54968 | -13.69403 | 108.67852 | A1 | 60 | 0.00000 |
| 593 | 60 | LEU | C    | -37.86300 | -16.28607 | 110.90549 | A1 | 60 | 0.00000 |
| 594 | 60 | LEU | O    | -36.81366 | -15.71151 | 110.64266 | A1 | 60 | 0.00000 |
| 595 | 61 | ALA | N    | -37.92548 | -17.30628 | 111.76650 | A1 | 61 | 0.00000 |
| 596 | 61 | ALA | H    | -38.80416 | -17.70206 | 112.04737 | A1 | 61 | 0.00000 |
| 597 | 61 | ALA | CA   | -36.66060 | -17.86080 | 112.25036 | A1 | 61 | 0.00000 |
| 598 | 61 | ALA | CB   | -36.90091 | -18.87147 | 113.37402 | A1 | 61 | 0.00000 |
| 599 | 61 | ALA | C    | -35.86652 | -18.52303 | 111.13575 | A1 | 61 | 0.00000 |
| 600 | 61 | ALA | O    | -34.67753 | -18.28483 | 110.93578 | A1 | 61 | 0.00000 |
| 601 | 62 | ASN | N    | -36.59182 | -19.33011 | 110.35468 | A1 | 62 | 0.00000 |
| 602 | 62 | ASN | H    | -37.55651 | -19.52444 | 110.56450 | A1 | 62 | 0.00000 |
| 603 | 62 | ASN | CA   | -35.93048 | -19.97053 | 109.20954 | A1 | 62 | 0.00000 |
| 604 | 62 | ASN | CB   | -36.90608 | -20.83397 | 108.41185 | A1 | 62 | 0.00000 |
| 605 | 62 | ASN | CG   | -36.14296 | -21.97501 | 107.76767 | A1 | 62 | 0.00000 |
| 606 | 62 | ASN | OD1  | -35.90083 | -23.00051 | 108.38915 | A1 | 62 | 0.00000 |
| 607 | 62 | ASN | ND2  | -35.81296 | -21.80385 | 106.49294 | A1 | 62 | 0.00000 |
| 608 | 62 | ASN | HD21 | -35.71613 | -20.90910 | 106.04169 | A1 | 62 | 0.00000 |
| 609 | 62 | ASN | HD22 | -35.64736 | -22.62041 | 105.92778 | A1 | 62 | 0.00000 |
| 610 | 62 | ASN | C    | -35.27272 | -18.97317 | 108.27635 | A1 | 62 | 0.00000 |
| 611 | 62 | ASN | O    | -34.08577 | -19.05772 | 107.98073 | A1 | 62 | 0.00000 |
| 612 | 63 | ILE | N    | -36.07385 | -17.96130 | 107.91224 | A1 | 63 | 0.00000 |
| 613 | 63 | ILE | H    | -37.03805 | -17.97906 | 108.18770 | A1 | 63 | 0.00000 |
| 614 | 63 | ILE | CA   | -35.60960 | -16.86395 | 107.05550 | A1 | 63 | 0.00000 |
| 615 | 63 | ILE | CB   | -36.79680 | -15.88630 | 106.84927 | A1 | 63 | 0.00000 |
| 616 | 63 | ILE | CG2  | -36.71800 | -14.58751 | 107.66300 | A1 | 63 | 0.00000 |
| 617 | 63 | ILE | CG1  | -37.00443 | -15.60068 | 105.36486 | A1 | 63 | 0.00000 |
| 618 | 63 | ILE | CD   | -38.27181 | -14.79756 | 105.06416 | A1 | 63 | 0.00000 |
| 619 | 63 | ILE | C    | -34.32421 | -16.14412 | 107.48562 | A1 | 63 | 0.00000 |
| 620 | 63 | ILE | O    | -33.67028 | -15.43835 | 106.72047 | A1 | 63 | 0.00000 |
| 621 | 64 | ALA | N    | -33.97867 | -16.34078 | 108.76481 | A1 | 64 | 0.00000 |
| 622 | 64 | ALA | H    | -34.55914 | -16.88095 | 109.37800 | A1 | 64 | 0.00000 |
| 623 | 64 | ALA | CA   | -32.68252 | -15.86370 | 109.23001 | A1 | 64 | 0.00000 |
| 624 | 64 | ALA | CB   | -32.78414 | -15.37252 | 110.67448 | A1 | 64 | 0.00000 |
| 625 | 64 | ALA | C    | -31.55324 | -16.91956 | 109.13883 | A1 | 64 | 0.00000 |
| 626 | 64 | ALA | O    | -30.45701 | -16.65389 | 108.75412 | A1 | 64 | 0.00000 |
| 627 | 65 | VAL | N    | -31.96250 | -18.15367 | 109.50633 | A1 | 65 | 0.00000 |
| 628 | 65 | VAL | H    | -32.92093 | -18.37377 | 109.71401 | A1 | 65 | 0.00000 |
| 629 | 65 | VAL | CA   | -30.91507 | -19.17596 | 109.47932 | A1 | 65 | 0.00000 |
| 630 | 65 | VAL | CB   | -31.28412 | -20.41152 | 110.33210 | A1 | 65 | 0.00000 |
| 631 | 65 | VAL | CG1  | -31.53866 | -19.97521 | 111.77524 | A1 | 65 | 0.00000 |
| 632 | 65 | VAL | CG2  | -32.45603 | -21.23819 | 109.79675 | A1 | 65 | 0.00000 |
| 633 | 65 | VAL | C    | -30.45713 | -19.56758 | 108.08237 | A1 | 65 | 0.00000 |
| 634 | 65 | VAL | O    | -29.26568 | -19.71596 | 107.82437 | A1 | 65 | 0.00000 |
| 635 | 66 | ASP | N    | -31.42136 | -19.66037 | 107.15805 | A1 | 66 | 0.00000 |
| 636 | 66 | ASP | H    | -32.38553 | -19.45723 | 107.38932 | A1 | 66 | 0.00000 |

FIG. 11

09013077 012699

|     |    |     |      |           |           |           |    |    |         |
|-----|----|-----|------|-----------|-----------|-----------|----|----|---------|
| 637 | 66 | ASP | CA   | -31.0     | -19.93216 | 105.76795 | A1 | 66 | 0.00000 |
| 638 | 66 | ASP | CB   | -32.31036 | -20.24966 | 104.93007 | A1 | 66 | 0.00000 |
| 639 | 66 | ASP | CG   | -33.44297 | -19.24219 | 105.08208 | A1 | 66 | 0.00000 |
| 640 | 66 | ASP | D1   | -33.16986 | -18.05114 | 105.20729 | A1 | 66 | 0.00000 |
| 641 | 66 | ASP | OD2  | -34.60286 | -19.65468 | 103.08126 | A1 | 66 | 0.00000 |
| 642 | 66 | ASP | C    | -30.18178 | -18.83449 | 105.15564 | A1 | 66 | 0.00000 |
| 643 | 66 | ASP | O    | -29.16482 | -19.06872 | 104.50705 | A1 | 66 | 0.00000 |
| 644 | 67 | LYS | N    | -30.56424 | -17.59916 | 105.48017 | A1 | 67 | 0.00000 |
| 645 | 67 | LYS | H    | -31.49538 | -17.48655 | 105.84055 | A1 | 67 | 0.00000 |
| 646 | 67 | LYS | CA   | -29.72959 | -16.43204 | 105.19320 | A1 | 67 | 0.00000 |
| 647 | 67 | LYS | CB   | -30.39071 | -15.23196 | 105.87104 | A1 | 67 | 0.00000 |
| 648 | 67 | LYS | CG   | -29.79159 | -13.86177 | 105.56853 | A1 | 67 | 0.00000 |
| 649 | 67 | LYS | CD   | -30.51506 | -12.79056 | 106.38164 | A1 | 67 | 0.00000 |
| 650 | 67 | LYS | CE   | -29.96446 | -11.38645 | 106.14720 | A1 | 67 | 0.00000 |
| 651 | 67 | LYS | NZ   | -30.60526 | -10.44891 | 107.01869 | A1 | 67 | 0.00000 |
| 652 | 67 | LYS | H21  | -30.33262 | -9.48398  | 106.85909 | A1 | 67 | 0.00000 |
| 653 | 67 | LYS | H22  | -31.70143 | -10.49161 | 106.80064 | A1 | 67 | 0.00000 |
| 654 | 67 | LYS | H23  | -30.53221 | -10.71804 | 108.01156 | A1 | 67 | 0.00000 |
| 655 | 67 | LYS | C    | -20.28117 | -16.58093 | 105.64383 | A1 | 67 | 0.00000 |
| 656 | 67 | LYS | O    | -27.33559 | -16.44078 | 104.87661 | A1 | 67 | 0.00000 |
| 657 | 68 | ALA | N    | -28.12520 | -16.92373 | 106.92795 | A1 | 68 | 0.00000 |
| 658 | 68 | ALA | H    | -28.92119 | -17.00935 | 107.53692 | A1 | 68 | 0.00000 |
| 659 | 68 | ALA | CA   | -26.76352 | -17.18143 | 107.40958 | A1 | 68 | 0.00000 |
| 660 | 68 | ALA | CB   | -26.77377 | -17.44846 | 108.91534 | A1 | 68 | 0.00000 |
| 661 | 68 | ALA | C    | -26.07149 | -18.34364 | 106.70618 | A1 | 68 | 0.00000 |
| 662 | 68 | ALA | O    | -24.80989 | -18.33297 | 106.37143 | A1 | 68 | 0.00000 |
| 663 | 69 | ASN | N    | -26.87877 | -19.37475 | 106.44973 | A1 | 69 | 0.00000 |
| 664 | 69 | ASN | H    | -27.84416 | -19.34421 | 106.72158 | A1 | 69 | 0.00000 |
| 665 | 69 | ASN | CA   | -26.32826 | -20.54731 | 105.77098 | A1 | 69 | 0.00000 |
| 666 | 69 | ASN | CB   | -27.33794 | -21.70567 | 105.74618 | A1 | 69 | 0.00000 |
| 667 | 69 | ASN | CG   | -27.75534 | -22.20215 | 107.12937 | A1 | 69 | 0.00000 |
| 668 | 69 | ASN | OD1  | -28.81753 | -22.77967 | 107.30600 | A1 | 69 | 0.00000 |
| 669 | 69 | ASN | ND2  | -26.90880 | -21.98927 | 108.13718 | A1 | 69 | 0.00000 |
| 670 | 69 | ASN | HD21 | -26.02949 | -21.53117 | 108.03476 | A1 | 69 | 0.00000 |
| 671 | 69 | ASN | HD22 | -27.17968 | -22.29754 | 109.04652 | A1 | 69 | 0.00000 |
| 672 | 69 | ASN | C    | -25.83413 | -20.26827 | 104.36379 | A1 | 69 | 0.00000 |
| 673 | 69 | ASN | O    | -24.88019 | -20.87816 | 103.89106 | A1 | 69 | 0.00000 |
| 674 | 70 | LEU | N    | -26.46696 | -19.27268 | 103.71664 | A1 | 70 | 0.00000 |
| 675 | 70 | LEU | H    | -27.27121 | -18.83110 | 104.12686 | A1 | 70 | 0.00000 |
| 676 | 70 | LEU | CA   | -25.93555 | -18.80513 | 102.42930 | A1 | 70 | 0.00000 |
| 677 | 70 | LEU | CB   | -26.70466 | -17.57714 | 101.93156 | A1 | 70 | 0.00000 |
| 678 | 70 | LEU | CG   | -28.07464 | -17.87907 | 101.32608 | A1 | 70 | 0.00000 |
| 679 | 70 | LEU | CD1  | -28.90878 | -16.60756 | 101.23109 | A1 | 70 | 0.00000 |
| 680 | 70 | LEU | CD2  | -27.93286 | -18.56192 | 99.96378  | A1 | 70 | 0.00000 |
| 681 | 70 | LEU | C    | -24.47328 | -18.42736 | 102.51389 | A1 | 70 | 0.00000 |
| 682 | 70 | LEU | O    | -23.64160 | -18.86456 | 101.72791 | A1 | 70 | 0.00000 |
| 683 | 71 | GLU | N    | -24.17065 | -17.62592 | 103.54240 | A1 | 71 | 0.00000 |
| 684 | 71 | GLU | H    | -24.87529 | -17.33320 | 104.19342 | A1 | 71 | 0.00000 |
| 685 | 71 | GLU | CA   | -22.77384 | -17.24207 | 103.73624 | A1 | 71 | 0.00000 |
| 686 | 71 | GLU | CB   | -22.68099 | -16.23884 | 104.88750 | A1 | 71 | 0.00000 |
| 687 | 71 | GLU | CG   | -21.33647 | -15.50613 | 104.93364 | A1 | 71 | 0.00000 |
| 688 | 71 | GLU | CD   | -21.30052 | -14.53829 | 106.10023 | A1 | 71 | 0.00000 |
| 689 | 71 | GLU | OE1  | -20.27115 | -14.47665 | 106.76570 | A1 | 71 | 0.00000 |
| 690 | 71 | GLU | OE2  | -22.29376 | -13.85012 | 106.33423 | A1 | 71 | 0.00000 |
| 691 | 71 | GLU | C    | -21.86369 | -18.43008 | 103.97868 | A1 | 71 | 0.00000 |
| 692 | 71 | GLU | O    | -20.81243 | -18.61050 | 103.36820 | A1 | 71 | 0.00000 |
| 693 | 72 | ILE | N    | -22.34609 | -19.31836 | 104.86364 | A1 | 72 | 0.00000 |
| 694 | 72 | ILE | H    | -23.21301 | -19.12129 | 105.33200 | A1 | 72 | 0.00000 |
| 695 | 72 | ILE | CA   | -21.56703 | -20.53142 | 105.13649 | A1 | 72 | 0.00000 |
| 696 | 72 | ILE | CB   | -22.29516 | -21.40405 | 106.17923 | A1 | 72 | 0.00000 |
| 697 | 72 | ILE | CG2  | -21.51796 | -22.60646 | 106.50604 | A1 | 72 | 0.00000 |
| 698 | 72 | ILE | CG1  | -22.55172 | -20.55465 | 107.45409 | A1 | 72 | 0.00000 |
| 699 | 72 | ILE | CD   | -23.34520 | -21.36278 | 108.51180 | A1 | 72 | 0.00000 |
| 700 | 72 | ILE | C    | -21.22106 | -21.35113 | 103.89490 | A1 | 72 | 0.00000 |

FIG. 12

000107.012698

|     |    |     |      |           |           |           |    |    |         |
|-----|----|-----|------|-----------|-----------|-----------|----|----|---------|
| 701 | 72 | ILE | O    | -20.79    | -21.68162 | 103.64178 | A1 | 72 | 0.00000 |
| 702 | 73 | MET | N    | -22.2.406 | -21.67127 | 103.09738 | A1 | 73 | 0.00000 |
| 703 | 73 | MET | H    | -23.17806 | -21.34412 | 103.27303 | A1 | 73 | 0.00000 |
| 704 | 73 | MET | CA   | -21.88577 | -22.51146 | 101.95532 | A1 | 73 | 0.00000 |
| 705 | 73 | MET | CB   | -23.02917 | -23.44601 | 101.56487 | A1 | 73 | 0.00000 |
| 706 | 73 | MET | CG   | -23.30745 | -24.44882 | 102.69030 | A1 | 73 | 0.00000 |
| 707 | 73 | MET | SD   | -24.39480 | -25.79652 | 102.19686 | A1 | 73 | 0.00000 |
| 708 | 73 | MET | CE   | -24.58745 | -26.56731 | 103.81212 | A1 | 73 | 0.00000 |
| 709 | 73 | MET | C    | -21.30840 | -21.79430 | 100.75010 | A1 | 73 | 0.00000 |
| 710 | 73 | MET | O    | -20.54740 | -22.36938 | 99.97894  | A1 | 73 | 0.00000 |
| 711 | 74 | THR | N    | -21.60342 | -20.49214 | 100.63510 | A1 | 74 | 0.00000 |
| 712 | 74 | THR | H    | -22.28955 | -20.04403 | 101.21510 | A1 | 74 | 0.00000 |
| 713 | 74 | THR | CA   | -20.82593 | -19.73833 | 99.64704  | A1 | 74 | 0.00000 |
| 714 | 74 | THR | CB   | -21.46299 | -18.35496 | 99.36040  | A1 | 74 | 0.00000 |
| 715 | 74 | THR | OG1  | -21.01301 | -17.84761 | 98.09669  | A1 | 74 | 0.00000 |
| 716 | 74 | THR | HG1  | -20.04699 | -17.88381 | 98.02785  | A1 | 74 | 0.00000 |
| 717 | 74 | THR | CG2  | -21.20740 | -17.31089 | 100.44667 | A1 | 74 | 0.00000 |
| 718 | 74 | THR | C    | -19.35170 | -19.61359 | 100.02467 | A1 | 74 | 0.00000 |
| 719 | 74 | THR | O    | -18.48554 | -19.49348 | 99.16750  | A1 | 74 | 0.00000 |
| 720 | 75 | LYS | N    | -19.08538 | -19.69260 | 101.33717 | A1 | 75 | 0.00000 |
| 721 | 75 | LYS | H    | -19.81675 | -19.65220 | 102.02321 | A1 | 75 | 0.00000 |
| 722 | 75 | LYS | CA   | -17.69833 | -19.83955 | 101.77078 | A1 | 75 | 0.00000 |
| 723 | 75 | LYS | CB   | -17.61408 | -19.57287 | 103.27797 | A1 | 75 | 0.00000 |
| 724 | 75 | LYS | CG   | -16.20208 | -19.66153 | 103.86107 | A1 | 75 | 0.00000 |
| 725 | 75 | LYS | CD   | -16.21091 | -19.57437 | 105.38567 | A1 | 75 | 0.00000 |
| 726 | 75 | LYS | CE   | -14.81504 | -19.74395 | 105.98417 | A1 | 75 | 0.00000 |
| 727 | 75 | LYS | N2   | -14.91179 | -19.69891 | 107.44939 | A1 | 75 | 0.00000 |
| 728 | 75 | LYS | H21  | -13.96620 | -19.83508 | 107.86470 | A1 | 75 | 0.00000 |
| 729 | 75 | LYS | H22  | -15.29159 | -18.77551 | 107.74094 | A1 | 75 | 0.00000 |
| 730 | 75 | LYS | H23  | -15.54844 | -20.45311 | 107.77639 | A1 | 75 | 0.00000 |
| 731 | 75 | LYS | C    | -17.14118 | -21.21778 | 101.45102 | A1 | 75 | 0.00000 |
| 732 | 75 | LYS | O    | -16.11623 | -21.36022 | 100.79660 | A1 | 75 | 0.00000 |
| 733 | 76 | ARG | N    | -17.86151 | -22.25466 | 101.90990 | A1 | 76 | 0.00000 |
| 734 | 76 | ARG | H    | -18.69512 | -22.09296 | 102.44436 | A1 | 76 | 0.00000 |
| 735 | 76 | ARG | CA   | -17.35520 | -23.61422 | 101.67525 | A1 | 76 | 0.00000 |
| 736 | 76 | ARG | CB   | -18.33654 | -24.60494 | 102.17145 | A1 | 76 | 0.00000 |
| 737 | 76 | ARG | CG   | -18.82789 | -24.66219 | 103.62361 | A1 | 76 | 0.00000 |
| 738 | 76 | ARG | CD   | -19.55383 | -25.98411 | 103.91795 | A1 | 76 | 0.00000 |
| 739 | 76 | ARG | NE   | -20.36155 | -25.99642 | 105.14334 | A1 | 76 | 0.00000 |
| 740 | 76 | ARG | HE   | -21.34527 | -25.85364 | 105.02467 | A1 | 76 | 0.00000 |
| 741 | 76 | ARG | CZ   | -19.85069 | -26.28686 | 106.34915 | A1 | 76 | 0.00000 |
| 742 | 76 | ARG | NH1  | -20.67426 | -26.45770 | 107.38550 | A1 | 76 | 0.00000 |
| 743 | 76 | ARG | NH11 | -20.32038 | -26.64144 | 108.30551 | A1 | 76 | 0.00000 |
| 744 | 76 | ARG | NH12 | -21.67206 | -26.42100 | 107.26619 | A1 | 76 | 0.00000 |
| 745 | 76 | ARG | NH2  | -18.53304 | -26.41209 | 106.51158 | A1 | 76 | 0.00000 |
| 746 | 76 | ARG | NH21 | -18.12377 | -26.62371 | 107.39854 | A1 | 76 | 0.00000 |
| 747 | 76 | ARG | NH22 | -17.92942 | -26.29542 | 105.72237 | A1 | 76 | 0.00000 |
| 748 | 76 | ARG | C    | -17.06072 | -23.91761 | 100.20901 | A1 | 76 | 0.00000 |
| 749 | 76 | ARG | O    | -16.02715 | -24.45819 | 99.83552  | A1 | 76 | 0.00000 |
| 750 | 77 | SER | N    | -18.01091 | -23.50462 | 99.36716  | A1 | 77 | 0.00000 |
| 751 | 77 | SER | H    | -18.84286 | -23.05363 | 99.69917  | A1 | 77 | 0.00000 |
| 752 | 77 | SER | CA   | -17.80506 | -23.71642 | 97.95702  | A1 | 77 | 0.00000 |
| 753 | 77 | SER | CB   | -19.13837 | -24.15898 | 97.32351  | A1 | 77 | 0.00000 |
| 754 | 77 | SER | OG   | -18.92403 | -25.08061 | 96.24728  | A1 | 77 | 0.00000 |
| 755 | 77 | SER | HG   | -18.99574 | -24.62840 | 95.39572  | A1 | 77 | 0.00000 |
| 756 | 77 | SER | C    | -17.22854 | -22.51234 | 97.20137  | A1 | 77 | 0.00000 |
| 757 | 77 | SER | O    | -17.39865 | -22.33993 | 96.00106  | A1 | 77 | 0.00000 |
| 758 | 78 | ASN | N    | -16.52714 | -21.66944 | 97.97646  | A1 | 78 | 0.00000 |
| 759 | 78 | ASN | H    | -16.44843 | -21.84082 | 98.96113  | A1 | 78 | 0.00000 |
| 760 | 78 | ASN | CA   | -15.74721 | -20.53857 | 97.45264  | A1 | 78 | 0.00000 |
| 761 | 78 | ASN | CB   | -14.33390 | -21.01377 | 97.09195  | A1 | 78 | 0.00000 |
| 762 | 78 | ASN | CG   | -13.52905 | -21.21984 | 98.36114  | A1 | 78 | 0.00000 |
| 763 | 78 | ASN | CD1  | -12.89956 | -20.31632 | 98.85264  | A1 | 78 | 0.00000 |
| 764 | 78 | ASN | ND2  | -13.55264 | -22.45457 | 98.85326  | A1 | 78 | 0.00000 |

|     |    |     |      |           |   |           |          |    |    |         |
|-----|----|-----|------|-----------|---|-----------|----------|----|----|---------|
| 765 | 78 | ASN | HD21 | -14.0     | 2 | -23.19170 | 98.43678 | A1 | 78 | 0.00000 |
| 766 | 78 | ASN | HD22 | -13.0     | 1 | -22.65362 | 99.68493 | A1 | 78 | 0.00000 |
| 767 | 78 | ASN | C    | -16.34134 |   | -19.72172 | 96.31352 | A1 | 78 | 0.00000 |
| 768 | 78 | ASN | O    | -15.71478 |   | -19.42979 | 95.30178 | A1 | 78 | 0.00000 |
| 769 | 79 | TYR | N    | -17.59612 |   | -19.32597 | 96.52354 | A1 | 79 | 0.00000 |
| 770 | 79 | TYR | H    | -18.05424 |   | -19.55771 | 97.38252 | A1 | 79 | 0.00000 |
| 771 | 79 | TYR | CA   | -18.21408 |   | -18.48918 | 95.49858 | A1 | 79 | 0.00000 |
| 772 | 79 | TYR | CB   | -19.64874 |   | -18.92649 | 95.21260 | A1 | 79 | 0.00000 |
| 773 | 79 | TYR | CG   | -19.74485 |   | -20.32764 | 94.65360 | A1 | 79 | 0.00000 |
| 774 | 79 | TYR | CD1  | -20.64246 |   | -21.23278 | 95.25950 | A1 | 79 | 0.00000 |
| 775 | 79 | TYR | CE1  | -20.76017 |   | -22.54189 | 94.75217 | A1 | 79 | 0.00000 |
| 776 | 79 | TYR | CD2  | -18.96361 |   | -20.72112 | 93.54108 | A1 | 79 | 0.00000 |
| 777 | 79 | TYR | CE2  | -19.07884 |   | -22.03339 | 93.03642 | A1 | 79 | 0.00000 |
| 778 | 79 | TYR | CZ   | -19.97533 |   | -22.93822 | 93.64752 | A1 | 79 | 0.00000 |
| 779 | 79 | TYR | OH   | -20.07585 |   | -24.23438 | 93.18578 | A1 | 79 | 0.00000 |
| 780 | 79 | TYR | HH   | -19.67682 |   | -24.30670 | 92.31232 | A1 | 79 | 0.00000 |
| 781 | 79 | TYR | C    | -18.21035 |   | -17.01261 | 95.83719 | A1 | 79 | 0.00000 |
| 782 | 79 | TYR | O    | -18.85099 |   | -16.51273 | 96.76683 | A1 | 79 | 0.00000 |
| 783 | 80 | THR | N    | -17.42457 |   | -16.33235 | 95.00452 | A1 | 80 | 0.00000 |
| 784 | 80 | THR | H    | -16.96429 |   | -16.79509 | 94.24288 | A1 | 80 | 0.00000 |
| 785 | 80 | THR | CA   | -17.09577 |   | -14.92660 | 95.20513 | A1 | 80 | 0.00000 |
| 786 | 80 | THR | CB   | -15.89072 |   | -14.87711 | 96.18098 | A1 | 80 | 0.00000 |
| 787 | 80 | THR | OG1  | -15.49849 |   | -13.52440 | 96.43537 | A1 | 80 | 0.00000 |
| 788 | 80 | THR | HG1  | -14.60960 |   | -13.50159 | 96.80560 | A1 | 80 | 0.00000 |
| 789 | 80 | THR | CG2  | -14.69719 |   | -15.72265 | 95.72104 | A1 | 80 | 0.00000 |
| 790 | 80 | THR | C    | -16.77512 |   | -14.32258 | 93.03840 | A1 | 80 | 0.00000 |
| 791 | 80 | THR | O    | -16.16679 |   | -14.97644 | 92.99811 | A1 | 80 | 0.00000 |
| 792 | 81 | PRO | N    | -17.23243 |   | -13.08096 | 93.61451 | A1 | 81 | 0.00000 |
| 793 | 81 | PRO | CD   | -10.04687 |   | -12.25452 | 94.50529 | A1 | 81 | 0.00000 |
| 794 | 81 | PRO | CA   | -16.95963 |   | -12.43774 | 92.32255 | A1 | 81 | 0.00000 |
| 795 | 81 | PRO | CB   | -18.08102 |   | -11.39225 | 92.28996 | A1 | 81 | 0.00000 |
| 796 | 81 | PRO | CG   | -18.22970 |   | -10.94901 | 93.74456 | A1 | 81 | 0.00000 |
| 797 | 81 | PRO | C    | -15.57247 |   | -11.80328 | 92.25040 | A1 | 81 | 0.00000 |
| 798 | 81 | PRO | D    | -15.41926 |   | -10.58936 | 92.16776 | A1 | 81 | 0.00000 |
| 799 | 82 | ILE | N    | -14.55883 |   | -12.66988 | 92.27154 | A1 | 82 | 0.00000 |
| 800 | 82 | ILE | H    | -14.69364 |   | -13.66392 | 92.31920 | A1 | 82 | 0.00000 |
| 801 | 82 | ILE | CA   | -13.18946 |   | -12.18130 | 92.13921 | A1 | 82 | 0.00000 |
| 802 | 82 | ILE | CB   | -12.60010 |   | -11.87598 | 93.53959 | A1 | 82 | 0.00000 |
| 803 | 82 | ILE | CG2  | -12.41140 |   | -13.13773 | 94.38674 | A1 | 82 | 0.00000 |
| 804 | 82 | ILE | CG1  | -11.31152 |   | -11.05228 | 93.44331 | A1 | 82 | 0.00000 |
| 805 | 82 | ILE | CD   | -10.76554 |   | -10.62709 | 94.80896 | A1 | 82 | 0.00000 |
| 806 | 82 | ILE | C    | -12.35649 |   | -13.19907 | 91.37376 | A1 | 82 | 0.00000 |
| 807 | 82 | ILE | OCT1 | -11.36717 |   | -12.81747 | 90.75062 | A1 | 82 | 0.00000 |
| 808 | 82 | ILE | OCT2 | -12.72556 |   | -14.37446 | 91.38671 | A1 | 82 | 0.00000 |
| 809 | 83 | GLY | N    | -17.53322 |   | -0.31236  | 94.99084 | B1 | 1  | 0.00000 |
| 810 | 83 | GLY | HT1  | -17.21994 |   | 0.44323   | 94.35235 | B1 | 1  | 0.00000 |
| 811 | 83 | GLY | HT2  | -16.86357 |   | -1.12219  | 94.96444 | B1 | 1  | 0.00000 |
| 812 | 83 | GLY | HT3  | -17.61098 |   | 0.01920   | 95.97150 | B1 | 1  | 0.00000 |
| 813 | 83 | GLY | CA   | -18.79853 |   | -0.91116  | 94.55151 | B1 | 1  | 0.00000 |
| 814 | 83 | GLY | C    | -18.52573 |   | -2.38203  | 94.66351 | B1 | 1  | 0.00000 |
| 815 | 83 | GLY | O    | -17.35786 |   | -2.70920  | 94.84086 | B1 | 1  | 0.00000 |
| 816 | 84 | ASP | N    | -19.57260 |   | -3.20239  | 94.59303 | B1 | 2  | 0.00000 |
| 817 | 84 | ASP | H    | -20.49658 |   | -2.89510  | 94.35600 | B1 | 2  | 0.00000 |
| 818 | 84 | ASP | CA   | -19.43900 |   | -4.63200  | 94.86181 | B1 | 2  | 0.00000 |
| 819 | 84 | ASP | CB   | -19.44643 |   | -4.83356  | 96.38475 | B1 | 2  | 0.00000 |
| 820 | 84 | ASP | CG   | -18.89301 |   | -6.19619  | 96.73815 | B1 | 2  | 0.00000 |
| 821 | 84 | ASP | OD1  | -17.69451 |   | -6.29764  | 96.98109 | B1 | 2  | 0.00000 |
| 822 | 84 | ASP | OD2  | -19.66566 |   | -7.14958  | 96.75715 | B1 | 2  | 0.00000 |
| 823 | 84 | ASP | C    | -20.62786 |   | -5.31072  | 94.19848 | B1 | 2  | 0.00000 |
| 824 | 84 | ASP | O    | -21.46903 |   | -4.61697  | 93.63479 | B1 | 2  | 0.00000 |
| 825 | 85 | THR | N    | -20.67796 |   | -6.64606  | 94.24891 | B1 | 3  | 0.00000 |
| 826 | 85 | THR | H    | -20.04362 |   | -7.15926  | 94.84032 | B1 | 3  | 0.00000 |
| 827 | 85 | THR | CA   | -21.75257 |   | -7.39367  | 93.59154 | B1 | 3  | 0.00000 |
| 828 | 85 | THR | CB   | -21.58903 |   | -7.31940  | 92.05122 | B1 | 3  | 0.00000 |

FIG. 14

00013077 012698

09043077 012698

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|     |    |     |      |           |           |           |    |   |         |
|-----|----|-----|------|-----------|-----------|-----------|----|---|---------|
| 829 | 85 | THR | OG1  | -22.165   | -7.82400  | 91.39964  | B1 | 3 | 0.00000 |
| 830 | 85 | THR | HG1  | -22.73431 | -7.60152  | 90.46343  | B1 | 3 | 0.00000 |
| 831 | 85 | THR | CG2  | -20.32966 | -8.02078  | 91.53071  | B1 | 3 | 0.00000 |
| 832 | 85 | THR | C    | -21.74290 | -8.83241  | 94.09035  | B1 | 3 | 0.00000 |
| 833 | 85 | THR | O    | -20.76454 | -9.30377  | 94.65381  | B1 | 3 | 0.00000 |
| 834 | 86 | ARG | N    | -22.86491 | -9.52779  | 93.88799  | B1 | 4 | 0.00000 |
| 835 | 86 | ARG | H    | -23.62404 | -9.13760  | 93.36423  | B1 | 4 | 0.00000 |
| 836 | 86 | ARG | CA   | -22.93360 | -10.87552 | 94.44830  | B1 | 4 | 0.00000 |
| 837 | 86 | ARG | CB   | -23.51668 | -10.79083 | 95.86916  | B1 | 4 | 0.00000 |
| 838 | 86 | ARG | CG   | -22.74323 | -11.65365 | 96.87092  | B1 | 4 | 0.00000 |
| 839 | 86 | ARG | CD   | -23.23116 | -13.10294 | 97.02541  | B1 | 4 | 0.00000 |
| 840 | 86 | ARG | NE   | -22.12580 | -14.03911 | 97.27083  | B1 | 4 | 0.00000 |
| 841 | 86 | ARG | HE   | -21.93083 | -14.68836 | 96.53494  | B1 | 4 | 0.00000 |
| 842 | 86 | ARG | CZ   | -21.37502 | -14.05016 | 98.38612  | B1 | 4 | 0.00000 |
| 843 | 86 | ARG | NH1  | -20.31371 | -14.85617 | 98.44757  | B1 | 4 | 0.00000 |
| 844 | 86 | ARG | NH11 | -19.73815 | -14.87872 | 99.26299  | B1 | 4 | 0.00000 |
| 845 | 86 | ARG | NH12 | -20.05194 | -15.47498 | 97.69021  | B1 | 4 | 0.00000 |
| 846 | 86 | ARG | NH2  | -21.67517 | -13.26636 | 99.42563  | B1 | 4 | 0.00000 |
| 847 | 86 | ARG | NH21 | -21.13780 | -13.26659 | 100.26897 | B1 | 4 | 0.00000 |
| 848 | 86 | ARG | NH22 | -22.46145 | -12.65025 | 99.36831  | B1 | 4 | 0.00000 |
| 849 | 86 | ARG | C    | -23.73522 | -11.82065 | 93.57905  | B1 | 4 | 0.00000 |
| 850 | 86 | ARG | O    | -24.85200 | -11.52803 | 93.17882  | B1 | 4 | 0.00000 |
| 851 | 87 | PRO | N    | -23.12190 | -12.98532 | 93.27325  | B1 | 5 | 0.00000 |
| 852 | 87 | PRO | CD   | -21.73269 | -13.34562 | 93.54376  | B1 | 5 | 0.00000 |
| 853 | 87 | PRO | CA   | -23.84435 | -14.02757 | 92.53087  | B1 | 5 | 0.00000 |
| 854 | 87 | PRO | CB   | -22.76528 | -15.13066 | 92.39999  | B1 | 5 | 0.00000 |
| 855 | 87 | PRO | CG   | -21.43460 | -14.43376 | 92.52460  | B1 | 5 | 0.00000 |
| 856 | 87 | PRO | C    | -25.10390 | -14.54496 | 93.21975  | B1 | 5 | 0.00000 |
| 857 | 87 | PRO | O    | -25.32441 | -14.39544 | 94.41838  | B1 | 5 | 0.00000 |
| 858 | 88 | ARG | N    | -25.94344 | -15.17061 | 92.39123  | B1 | 6 | 0.00000 |
| 859 | 88 | ARG | H    | -25.68611 | -15.35588 | 91.44433  | B1 | 6 | 0.00000 |
| 860 | 88 | ARG | CA   | -27.23219 | -15.62675 | 92.90235  | B1 | 6 | 0.00000 |
| 861 | 88 | ARG | CB   | -28.29078 | -15.39805 | 91.81653  | B1 | 6 | 0.00000 |
| 862 | 88 | ARG | CG   | -29.70863 | -15.55859 | 92.35844  | B1 | 6 | 0.00000 |
| 863 | 88 | ARG | CD   | -30.79150 | -14.91787 | 91.49236  | B1 | 6 | 0.00000 |
| 864 | 88 | ARG | NE   | -31.92741 | -14.57277 | 92.34607  | B1 | 6 | 0.00000 |
| 865 | 88 | ARG | HE   | -31.76512 | -14.64038 | 93.33788  | B1 | 6 | 0.00000 |
| 866 | 88 | ARG | CZ   | -33.08881 | -14.12165 | 91.86193  | B1 | 6 | 0.00000 |
| 867 | 88 | ARG | NH1  | -34.06565 | -13.81756 | 92.71322  | B1 | 6 | 0.00000 |
| 868 | 88 | ARG | NH11 | -34.95441 | -13.48157 | 92.40144  | B1 | 6 | 0.00000 |
| 869 | 88 | ARG | NH12 | -33.91853 | -13.92533 | 93.69838  | B1 | 6 | 0.00000 |
| 870 | 88 | ARG | NH2  | -33.26623 | -13.97383 | 90.54974  | B1 | 6 | 0.00000 |
| 871 | 88 | ARG | NH21 | -34.12737 | -13.64013 | 90.16725  | B1 | 6 | 0.00000 |
| 872 | 88 | ARG | NH22 | -32.52080 | -14.19859 | 89.92214  | B1 | 6 | 0.00000 |
| 873 | 88 | ARG | C    | -27.23157 | -17.07404 | 93.36366  | B1 | 6 | 0.00000 |
| 874 | 88 | ARG | O    | -26.89591 | -18.00090 | 92.63574  | B1 | 6 | 0.00000 |
| 875 | 89 | PHE | N    | -27.62757 | -17.24057 | 94.62546  | B1 | 7 | 0.00000 |
| 876 | 89 | PHE | H    | -27.92346 | -16.46797 | 95.18173  | B1 | 7 | 0.00000 |
| 877 | 89 | PHE | CA   | -27.64368 | -18.59443 | 95.17433  | B1 | 7 | 0.00000 |
| 878 | 89 | PHE | CB   | -26.56379 | -18.74887 | 96.25427  | B1 | 7 | 0.00000 |
| 879 | 89 | PHE | CG   | -25.20774 | -18.55805 | 95.61829  | B1 | 7 | 0.00000 |
| 880 | 89 | PHE | CD1  | -24.74915 | -19.48139 | 94.64858  | B1 | 7 | 0.00000 |
| 881 | 89 | PHE | CD2  | -24.42840 | -17.43023 | 95.96102  | B1 | 7 | 0.00000 |
| 882 | 89 | PHE | CE1  | -23.51045 | -19.27079 | 94.00961  | B1 | 7 | 0.00000 |
| 883 | 89 | PHE | CE2  | -23.18767 | -17.21576 | 95.32384  | B1 | 7 | 0.00000 |
| 884 | 89 | PHE | CZ   | -22.73800 | -18.13927 | 94.34976  | B1 | 7 | 0.00000 |
| 885 | 89 | PHE | C    | -28.99632 | -18.97147 | 95.72084  | B1 | 7 | 0.00000 |
| 886 | 89 | PHE | O    | -29.85551 | -18.12429 | 95.94786  | B1 | 7 | 0.00000 |
| 887 | 90 | LEU | N    | -29.15750 | -20.28822 | 95.87791  | B1 | 8 | 0.00000 |
| 888 | 90 | LEU | H    | -26.38720 | -20.92114 | 95.76376  | B1 | 8 | 0.00000 |
| 889 | 90 | LEU | CA   | -30.48575 | -20.02226 | 96.14113  | B1 | 8 | 0.00000 |
| 890 | 90 | LEU | CB   | -31.01268 | -21.46546 | 94.64961  | B1 | 8 | 0.00000 |
| 891 | 90 | LEU | CG   | -32.46079 | -21.16892 | 94.43614  | B1 | 8 | 0.00000 |
| 892 | 90 | LEU | CD1  | -32.81113 | -21.98230 | 93.19113  | B1 | 8 | 0.00000 |

FIG. 15

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DR1\_MIN2.CRD

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|     |    |     |       |           |   |           |           |    |    |         |
|-----|----|-----|-------|-----------|---|-----------|-----------|----|----|---------|
| 893 | 90 | LEU | CD2   | -33.4     | 8 | -21.40699 | 95.55222  | B1 | 8  | 0.00000 |
| 894 | 90 | LEU | C     | -30.45467 |   | -21.90281 | 97.20252  | B1 | 8  | 0.00000 |
| 895 | 90 | LEU | O     | -29.74216 |   | -22.89200 | 97.07224  | B1 | 8  | 0.00000 |
| 896 | 91 | TRP | N     | -31.28133 |   | -21.71086 | 98.22982  | B1 | 9  | 0.00000 |
| 897 | 91 | TRP | H     | -31.78897 |   | -20.85226 | 98.31900  | B1 | 9  | 0.00000 |
| 898 | 91 | TRP | CA    | -31.61477 |   | -22.06043 | 99.06700  | B1 | 9  | 0.00000 |
| 899 | 91 | TRP | CB    | -31.76159 |   | -22.50789 | 100.54418 | B1 | 9  | 0.00000 |
| 900 | 91 | TRP | CG    | -30.46050 |   | -22.11490 | 101.18157 | B1 | 9  | 0.00000 |
| 901 | 91 | TRP | CD2   | -29.22893 |   | -22.79283 | 101.16170 | B1 | 9  | 0.00000 |
| 902 | 91 | TRP | CE2   | -28.30074 |   | -21.96546 | 101.98847 | B1 | 9  | 0.00000 |
| 903 | 91 | TRP | CE3   | -28.77368 |   | -24.00327 | 100.60389 | B1 | 9  | 0.00000 |
| 904 | 91 | TRP | CD1   | -30.26500 |   | -20.96427 | 101.96112 | B1 | 9  | 0.00000 |
| 905 | 91 | TRP | HE1   | -28.99810 |   | -20.87047 | 102.44030 | B1 | 9  | 0.00000 |
| 906 | 91 | TRP | HE1   | -28.68566 |   | -20.15616 | 103.04137 | B1 | 9  | 0.00000 |
| 907 | 91 | TRP | CZ2   | -26.97767 |   | -22.40520 | 102.16578 | B1 | 9  | 0.00000 |
| 908 | 91 | TRP | CZ3   | -27.44054 |   | -24.40402 | 100.81577 | B1 | 9  | 0.00000 |
| 909 | 91 | TRP | CH2   | -26.56124 |   | -23.61859 | 101.58828 | B1 | 9  | 0.00000 |
| 910 | 91 | TRP | C     | -32.96765 |   | -23.39534 | 98.70806  | B1 | 9  | 0.00000 |
| 911 | 91 | TRP | O     | -33.92486 |   | -22.66026 | 98.49798  | B1 | 9  | 0.00000 |
| 912 | 92 | GLN | N---- | -33.02847 |   | -24.71550 | 98.69197  | B1 | 10 | 0.00000 |
| 913 | 92 | GLN | H     | -32.20362 |   | -25.28365 | 98.76579  | B1 | 10 | 0.00000 |
| 914 | 92 | GLN | CA    | -34.33516 |   | -25.34751 | 98.65309  | B1 | 10 | 0.00000 |
| 915 | 92 | GLN | CB    | -34.50105 |   | -26.04119 | 97.30049  | B1 | 10 | 0.00000 |
| 916 | 92 | GLN | CG    | -34.43287 |   | -25.05724 | 96.13126  | B1 | 10 | 0.00000 |
| 917 | 92 | GLN | CD    | -34.12668 |   | -25.79390 | 94.84833  | B1 | 10 | 0.00000 |
| 918 | 92 | GLN | OE1   | -32.99424 |   | -25.68638 | 94.39010  | B1 | 10 | 0.00000 |
| 919 | 92 | GLN | NE2   | -35.19268 |   | -26.32196 | 94.25873  | B1 | 10 | 0.00000 |
| 920 | 92 | GLN | HE21  | -36.10617 |   | -26.21874 | 94.65013  | B1 | 10 | 0.00000 |
| 921 | 92 | GLN | HE22  | -35.08609 |   | -26.83019 | 93.40658  | B1 | 10 | 0.00000 |
| 922 | 92 | GLN | C     | -34.37000 |   | -26.35610 | 99.77327  | B1 | 10 | 0.00000 |
| 923 | 92 | GLN | O     | -33.40619 |   | -27.07419 | 100.00960 | B1 | 10 | 0.00000 |
| 924 | 93 | LEU | N     | -35.49484 |   | -26.39205 | 100.47380 | B1 | 11 | 0.00000 |
| 925 | 93 | LEU | H     | -36.24432 |   | -25.74963 | 100.29272 | B1 | 11 | 0.00000 |
| 926 | 93 | LEU | CA    | -35.59559 |   | -27.43909 | 101.48633 | B1 | 11 | 0.00000 |
| 927 | 93 | LEU | CB    | -35.41178 |   | -26.81504 | 102.88181 | B1 | 11 | 0.00000 |
| 928 | 93 | LEU | CG    | -34.83577 |   | -27.70766 | 103.99848 | B1 | 11 | 0.00000 |
| 929 | 93 | LEU | CD1   | -34.33031 |   | -26.83624 | 105.14843 | B1 | 11 | 0.00000 |
| 930 | 93 | LEU | CD2   | -35.82812 |   | -28.74167 | 104.52005 | B1 | 11 | 0.00000 |
| 931 | 93 | LEU | C     | -36.93596 |   | -28.11112 | 101.32695 | B1 | 11 | 0.00000 |
| 932 | 93 | LEU | O     | -37.91692 |   | -27.47571 | 100.96621 | B1 | 11 | 0.00000 |
| 933 | 94 | LYS | N     | -36.95045 |   | -29.41719 | 101.56549 | B1 | 12 | 0.00000 |
| 934 | 94 | LYS | H     | -36.10205 |   | -29.89066 | 101.79736 | B1 | 12 | 0.00000 |
| 935 | 94 | LYS | CA    | -38.21063 |   | -30.14121 | 101.49214 | B1 | 12 | 0.00000 |
| 936 | 94 | LYS | CB    | -38.26049 |   | -30.88530 | 100.13839 | B1 | 12 | 0.00000 |
| 937 | 94 | LYS | CG    | -39.43761 |   | -31.85442 | 100.07544 | B1 | 12 | 0.00000 |
| 938 | 94 | LYS | CD    | -39.91969 |   | -32.44832 | 98.75113  | B1 | 12 | 0.00000 |
| 939 | 94 | LYS | CE    | -41.00198 |   | -33.40442 | 99.23924  | B1 | 12 | 0.00000 |
| 940 | 94 | LYS | NZ    | -41.98389 |   | -33.90963 | 98.26846  | B1 | 12 | 0.00000 |
| 941 | 94 | LYS | HZ1   | -42.69798 |   | -34.41995 | 98.86351  | B1 | 12 | 0.00000 |
| 942 | 94 | LYS | HZ2   | -42.49249 |   | -33.14263 | 97.78947  | B1 | 12 | 0.00000 |
| 943 | 94 | LYS | HZ3   | -41.57162 |   | -34.57937 | 97.59540  | B1 | 12 | 0.00000 |
| 944 | 94 | LYS | C     | -38.34910 |   | -31.08699 | 102.67642 | B1 | 12 | 0.00000 |
| 945 | 94 | LYS | O     | -37.54720 |   | -31.99770 | 102.85849 | B1 | 12 | 0.00000 |
| 946 | 95 | PHE | N     | -39.40676 |   | -30.85529 | 103.46609 | B1 | 13 | 0.00000 |
| 947 | 95 | PHE | H     | -39.99321 |   | -30.05201 | 103.34519 | B1 | 13 | 0.00000 |
| 948 | 95 | PHE | CA    | -39.73794 |   | -31.84982 | 104.49053 | B1 | 13 | 0.00000 |
| 949 | 95 | PHE | CB    | -39.13251 |   | -31.49228 | 105.86481 | B1 | 13 | 0.00000 |
| 950 | 95 | PHE | CG    | -39.62104 |   | -30.20819 | 106.49960 | B1 | 13 | 0.00000 |
| 951 | 95 | PHE | CD1   | -39.04917 |   | -28.96886 | 106.12996 | B1 | 13 | 0.00000 |
| 952 | 95 | PHE | CD2   | -40.60668 |   | -30.26479 | 107.51173 | B1 | 13 | 0.00000 |
| 953 | 95 | PHE | CE1   | -39.45587 |   | -27.78326 | 106.77985 | B1 | 13 | 0.00000 |
| 954 | 95 | PHE | CE2   | -41.01477 |   | -29.08019 | 108.16313 | B1 | 13 | 0.00000 |
| 955 | 95 | PHE | CZ    | -40.43557 |   | -27.84435 | 107.79605 | B1 | 13 | 0.00000 |
| 956 | 95 | PHE | C     | -41.22005 |   | -32.16799 | 104.57423 | B1 | 13 | 0.00000 |

FIG. 16



|      |     |     |      |           |           |           |    |    |         |
|------|-----|-----|------|-----------|-----------|-----------|----|----|---------|
| 957  | 95  | PHE | O    | -42.0     | -31.31332 | 104.41691 | B1 | 13 | 0.00000 |
| 958  | 96  | GLU | N    | -41.47812 | -33.46734 | 104.75822 | B1 | 14 | 0.00000 |
| 959  | 96  | GLU | H    | -40.74093 | -34.09071 | 105.01948 | B1 | 14 | 0.00000 |
| 960  | 96  | GLU | CA   | -42.80002 | -33.99059 | 104.40078 | B1 | 14 | 0.00000 |
| 961  | 96  | GLU | CB   | -42.75085 | -34.25375 | 102.88321 | B1 | 14 | 0.00000 |
| 962  | 96  | GLU | CG   | -43.92070 | -34.87965 | 102.11791 | B1 | 14 | 0.00000 |
| 963  | 96  | GLU | CD   | -43.55505 | -34.92496 | 100.64018 | B1 | 14 | 0.00000 |
| 964  | 96  | GLU | OE1  | -44.08205 | -34.15253 | 99.84297  | B1 | 14 | 0.00000 |
| 965  | 96  | GLU | OE2  | -42.67962 | -35.68559 | 100.23154 | B1 | 14 | 0.00000 |
| 966  | 96  | GLU | C    | -43.13129 | -35.25393 | 105.17925 | B1 | 14 | 0.00000 |
| 967  | 96  | GLU | O    | -42.27510 | -36.11395 | 105.37879 | B1 | 14 | 0.00000 |
| 968  | 97  | CYS | N    | -44.39621 | -35.34431 | 105.62501 | B1 | 15 | 0.00000 |
| 969  | 97  | CYS | H    | -45.05281 | -34.60566 | 105.44206 | B1 | 15 | 0.00000 |
| 970  | 97  | CYS | CA   | -44.78990 | -36.60747 | 106.25700 | B1 | 15 | 0.00000 |
| 971  | 97  | CYS | CB   | -45.09404 | -36.46870 | 107.76554 | B1 | 15 | 0.00000 |
| 972  | 97  | CYS | SG   | -46.49873 | -35.54248 | 108.42288 | B1 | 15 | 0.00000 |
| 973  | 97  | CYS | C    | -45.89248 | -37.36966 | 105.55706 | B1 | 15 | 0.00000 |
| 974  | 97  | CYS | O    | -46.75253 | -36.80546 | 104.88787 | B1 | 15 | 0.00000 |
| 975  | 98  | HIS | N    | -45.80356 | -38.69951 | 105.71784 | B1 | 16 | 0.00000 |
| 976  | 98  | HIS | H    | -45.06854 | -39.11332 | 106.26371 | B1 | 16 | 0.00000 |
| 977  | 98  | HIS | CA   | -46.75592 | -39.59530 | 105.05785 | B1 | 16 | 0.00000 |
| 978  | 98  | HIS | CB   | -46.00867 | -40.61029 | 104.19437 | B1 | 16 | 0.00000 |
| 979  | 98  | HIS | CG   | -45.38253 | -39.98357 | 102.97364 | B1 | 16 | 0.00000 |
| 980  | 98  | HIS | ND1  | -45.88967 | -40.13539 | 101.74183 | B1 | 16 | 0.00000 |
| 981  | 98  | HIS | HD1  | -46.72307 | -40.60043 | 101.51181 | B1 | 16 | 0.00000 |
| 982  | 98  | HIS | CD2  | -44.21266 | -39.22166 | 102.89430 | B1 | 16 | 0.00000 |
| 983  | 98  | HIS | NE2  | -44.02276 | -38.92334 | 101.58753 | B1 | 16 | 0.00000 |
| 984  | 98  | HIS | CE1  | -45.05268 | -39.48062 | 100.87633 | B1 | 16 | 0.00000 |
| 985  | 98  | HIS | C    | -47.56750 | -40.40062 | 106.05217 | B1 | 16 | 0.00000 |
| 986  | 98  | HIS | O    | -47.04279 | -40.99638 | 106.99225 | B1 | 16 | 0.00000 |
| 987  | 99  | PHE | N    | -48.87987 | -40.39547 | 105.81218 | B1 | 17 | 0.00000 |
| 988  | 99  | PHE | H    | -49.25243 | -39.92869 | 105.00666 | B1 | 17 | 0.00000 |
| 989  | 99  | PHE | CA   | -49.78029 | -41.01889 | 106.77662 | B1 | 17 | 0.00000 |
| 990  | 99  | PHE | CB   | -50.48946 | -39.93190 | 107.59234 | B1 | 17 | 0.00000 |
| 991  | 99  | PHE | CG   | -49.63868 | -39.72312 | 108.81497 | B1 | 17 | 0.00000 |
| 992  | 99  | PHE | CD1  | -48.50685 | -38.87580 | 108.76543 | B1 | 17 | 0.00000 |
| 993  | 99  | PHE | CD2  | -49.92563 | -40.47457 | 109.97439 | B1 | 17 | 0.00000 |
| 994  | 99  | PHE | CE1  | -47.64103 | -38.80002 | 109.87537 | B1 | 17 | 0.00000 |
| 995  | 99  | PHE | CE2  | -49.06252 | -40.39779 | 111.08254 | B1 | 17 | 0.00000 |
| 996  | 99  | PHE | CZ   | -47.92137 | -39.56658 | 111.02626 | B1 | 17 | 0.00000 |
| 997  | 99  | PHE | C    | -50.79242 | -41.97404 | 106.19800 | B1 | 17 | 0.00000 |
| 998  | 99  | PHE | O    | -51.48007 | -41.71068 | 105.22101 | B1 | 17 | 0.00000 |
| 999  | 100 | PHE | N    | -50.86837 | -43.12653 | 106.85844 | B1 | 18 | 0.00000 |
| 1000 | 100 | PHE | H    | -50.32768 | -43.27017 | 107.68944 | B1 | 18 | 0.00000 |
| 1001 | 100 | PHE | CA   | -51.84718 | -44.10783 | 106.41132 | B1 | 18 | 0.00000 |
| 1002 | 100 | PHE | CB   | -51.44468 | -45.52210 | 106.84262 | B1 | 18 | 0.00000 |
| 1003 | 100 | PHE | CG   | -51.08740 | -46.34931 | 105.63001 | B1 | 18 | 0.00000 |
| 1004 | 100 | PHE | CD1  | -49.81159 | -46.95065 | 105.55366 | B1 | 18 | 0.00000 |
| 1005 | 100 | PHE | CD2  | -52.01269 | -46.50158 | 104.56911 | B1 | 18 | 0.00000 |
| 1006 | 100 | PHE | CE1  | -49.45012 | -47.69723 | 104.41336 | B1 | 18 | 0.00000 |
| 1007 | 100 | PHE | CE2  | -51.65494 | -47.24829 | 103.42719 | B1 | 18 | 0.00000 |
| 1008 | 100 | PHE | CZ   | -50.37408 | -47.83859 | 103.35608 | B1 | 18 | 0.00000 |
| 1009 | 100 | PHE | C    | -53.21727 | -43.84401 | 106.96975 | B1 | 18 | 0.00000 |
| 1010 | 100 | PHE | O    | -53.38235 | -43.49692 | 108.13319 | B1 | 18 | 0.00000 |
| 1011 | 101 | ASN | N    | -54.19611 | -44.08275 | 106.08672 | B1 | 19 | 0.00000 |
| 1012 | 101 | ASN | H    | -53.92777 | -44.28429 | 105.14366 | B1 | 19 | 0.00000 |
| 1013 | 101 | ASN | CA   | -55.63451 | -43.97453 | 106.37273 | B1 | 19 | 0.00000 |
| 1014 | 101 | ASN | CB   | -56.35400 | -45.03359 | 105.52094 | B1 | 19 | 0.00000 |
| 1015 | 101 | ASN | CG   | -57.86040 | -44.83624 | 105.52911 | B1 | 19 | 0.00000 |
| 1016 | 101 | ASN | OD1  | -58.43246 | -44.06601 | 104.77523 | B1 | 19 | 0.00000 |
| 1017 | 101 | ASN | ND2  | -58.51327 | -45.52184 | 106.41359 | B1 | 19 | 0.00000 |
| 1018 | 101 | ASN | HD21 | -58.04843 | -46.21753 | 107.02623 | B1 | 19 | 0.00000 |
| 1019 | 101 | ASN | HD22 | -59.50666 | -45.49785 | 106.46882 | B1 | 19 | 0.00000 |
| 1020 | 101 | ASN | C    | -56.06277 | -44.09262 | 107.83398 | B1 | 19 | 0.00000 |

FIG. 17

09013077.012698

09013077 012699

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|      |     |     |      |           |   |           |           |    |    |         |
|------|-----|-----|------|-----------|---|-----------|-----------|----|----|---------|
| 1021 | 101 | ASN | O    | -56.71    | 7 | -43.23997 | 108.39463 | B1 | 19 | 0.00000 |
| 1022 | 102 | GLY | N    | -55.61    | 0 | -45.10941 | 108.46454 | B1 | 20 | 0.00000 |
| 1023 | 102 | GLY | H    | -55.00370 |   | -45.02188 | 108.01935 | B1 | 20 | 0.00000 |
| 1024 | 102 | GLY | CA   | -55.97438 |   | -45.32353 | 109.88157 | B1 | 20 | 0.00000 |
| 1025 | 102 | GLY | C    | -55.02088 |   | -44.59872 | 110.81953 | B1 | 20 | 0.00000 |
| 1026 | 102 | GLY | O    | -54.46008 |   | -45.17864 | 111.73800 | B1 | 20 | 0.00000 |
| 1027 | 103 | THR | N    | -54.84744 |   | -43.29716 | 110.54648 | B1 | 21 | 0.00000 |
| 1028 | 103 | THR | H    | -55.35512 |   | -42.90731 | 109.77435 | B1 | 21 | 0.00000 |
| 1029 | 103 | THR | CA   | -53.96549 |   | -42.39542 | 111.30363 | B1 | 21 | 0.00000 |
| 1030 | 103 | THR | CB   | -54.75487 |   | -41.81263 | 112.51011 | B1 | 21 | 0.00000 |
| 1031 | 103 | THR | OG1  | -54.22405 |   | -40.53356 | 112.87483 | B1 | 21 | 0.00000 |
| 1032 | 103 | THR | HG1  | -54.81974 |   | -40.09919 | 113.49221 | B1 | 21 | 0.00000 |
| 1033 | 103 | THR | CG2  | -54.86925 |   | -42.72433 | 113.73959 | B1 | 21 | 0.00000 |
| 1034 | 103 | THR | C    | -52.56983 |   | -42.92386 | 111.66956 | B1 | 21 | 0.00000 |
| 1035 | 103 | THR | O    | -51.96086 |   | -42.59288 | 112.68707 | B1 | 21 | 0.00000 |
| 1036 | 104 | GLU | N    | -52.05837 |   | -43.78433 | 110.78327 | B1 | 22 | 0.00000 |
| 1037 | 104 | GLU | H    | -52.50836 |   | -43.94021 | 109.90068 | B1 | 22 | 0.00000 |
| 1038 | 104 | GLU | CA   | -50.80234 |   | -44.42458 | 111.16198 | B1 | 22 | 0.00000 |
| 1039 | 104 | GLU | CB   | -50.88647 |   | -45.95191 | 111.05395 | B1 | 22 | 0.00000 |
| 1040 | 104 | GLU | CG   | -51.13368 |   | -46.62525 | 112.41591 | B1 | 22 | 0.00000 |
| 1041 | 104 | GLU | CD   | -50.07267 |   | -46.21410 | 113.43075 | B1 | 22 | 0.00000 |
| 1042 | 104 | GLU | OE1  | -50.42273 |   | -45.91599 | 114.57130 | B1 | 22 | 0.00000 |
| 1043 | 104 | GLU | OE2  | -48.89658 |   | -46.13148 | 113.08359 | B1 | 22 | 0.00000 |
| 1044 | 104 | GLU | C    | -49.56607 |   | -43.91901 | 110.45954 | B1 | 22 | 0.00000 |
| 1045 | 104 | GLU | O    | -49.58628 |   | -43.40196 | 109.34894 | B1 | 22 | 0.00000 |
| 1046 | 105 | ARG | N    | -48.46470 |   | -44.04578 | 111.19345 | B1 | 23 | 0.00000 |
| 1047 | 105 | ARG | H    | -48.46820 |   | -44.67995 | 111.97754 | B1 | 23 | 0.00000 |
| 1048 | 105 | ARG | CA   | -47.23862 |   | -43.36578 | 110.79677 | B1 | 23 | 0.00000 |
| 1049 | 105 | ARG | CB   | -46.43619 |   | -43.14957 | 112.09184 | B1 | 23 | 0.00000 |
| 1050 | 105 | ARG | CG   | -45.11167 |   | -42.37595 | 112.05228 | B1 | 23 | 0.00000 |
| 1051 | 105 | ARG | CD   | -43.89570 |   | -43.22016 | 111.65081 | B1 | 23 | 0.00000 |
| 1052 | 105 | ARG | NE   | -42.65640 |   | -42.46704 | 111.89499 | B1 | 23 | 0.00000 |
| 1053 | 105 | ARG | HE   | -42.30777 |   | -42.45915 | 112.83941 | B1 | 23 | 0.00000 |
| 1054 | 105 | ARG | CZ   | -42.05554 |   | -41.77685 | 110.93892 | B1 | 23 | 0.00000 |
| 1055 | 105 | ARG | NH1  | -41.02352 |   | -41.00938 | 111.25165 | B1 | 23 | 0.00000 |
| 1056 | 105 | ARG | HH11 | -40.51476 |   | -40.49136 | 110.56874 | B1 | 23 | 0.00000 |
| 1057 | 105 | ARG | HH12 | -40.73208 |   | -40.92747 | 112.21979 | B1 | 23 | 0.00000 |
| 1058 | 105 | ARG | NH2  | -42.47661 |   | -41.82718 | 109.68286 | B1 | 23 | 0.00000 |
| 1059 | 105 | ARG | HH21 | -42.19810 |   | -41.15340 | 109.00310 | B1 | 23 | 0.00000 |
| 1060 | 105 | ARG | HH22 | -43.08503 |   | -42.57763 | 109.38941 | B1 | 23 | 0.00000 |
| 1061 | 105 | ARG | C    | -46.47373 |   | -44.13883 | 109.74376 | B1 | 23 | 0.00000 |
| 1062 | 105 | ARG | O    | -46.02105 |   | -45.25363 | 109.97034 | B1 | 23 | 0.00000 |
| 1063 | 106 | VAL | N    | -46.32863 |   | -43.51517 | 108.56827 | B1 | 24 | 0.00000 |
| 1064 | 106 | VAL | H    | -46.72693 |   | -42.61352 | 108.37187 | B1 | 24 | 0.00000 |
| 1065 | 106 | VAL | CA   | -45.53349 |   | -44.24499 | 107.58352 | B1 | 24 | 0.00000 |
| 1066 | 106 | VAL | CB   | -46.27081 |   | -44.39073 | 106.24298 | B1 | 24 | 0.00000 |
| 1067 | 106 | VAL | CG1  | -45.79579 |   | -45.65575 | 105.52366 | B1 | 24 | 0.00000 |
| 1068 | 106 | VAL | CG2  | -47.77990 |   | -44.41166 | 106.42922 | B1 | 24 | 0.00000 |
| 1069 | 106 | VAL | C    | -44.14065 |   | -43.66075 | 107.41554 | B1 | 24 | 0.00000 |
| 1070 | 106 | VAL | O    | -43.30354 |   | -43.80891 | 108.29696 | B1 | 24 | 0.00000 |
| 1071 | 107 | ARG | N    | -43.87314 |   | -42.98069 | 106.29416 | B1 | 25 | 0.00000 |
| 1072 | 107 | ARG | H    | -44.58452 |   | -42.69040 | 105.65671 | B1 | 25 | 0.00000 |
| 1073 | 107 | ARG | CA   | -42.49561 |   | -42.53115 | 106.12329 | B1 | 25 | 0.00000 |
| 1074 | 107 | ARG | CB   | -41.95685 |   | -43.01317 | 104.76032 | B1 | 25 | 0.00000 |
| 1075 | 107 | ARG | CG   | -41.96328 |   | -42.02619 | 103.58362 | B1 | 25 | 0.00000 |
| 1076 | 107 | ARG | CD   | -42.33357 |   | -42.66829 | 102.24883 | B1 | 25 | 0.00000 |
| 1077 | 107 | ARG | NE   | -43.76838 |   | -42.53515 | 102.23147 | B1 | 25 | 0.00000 |
| 1078 | 107 | ARG | HE   | -44.37946 |   | -42.14312 | 102.28284 | B1 | 25 | 0.00000 |
| 1079 | 107 | ARG | CZ   | -44.26510 |   | -44.17490 | 102.20945 | B1 | 25 | 0.00000 |
| 1080 | 107 | ARG | NH1  | -45.56598 |   | -44.32747 | 102.35905 | B1 | 25 | 0.00000 |
| 1081 | 107 | ARG | HH11 | -46.08629 |   | -45.19207 | 102.34562 | B1 | 25 | 0.00000 |
| 1082 | 107 | ARG | HH12 | -45.19539 |   | -43.55730 | 102.54612 | B1 | 25 | 0.00000 |
| 1083 | 107 | ARG | HH2  | -43.47983 |   | -45.23695 | 102.05793 | B1 | 25 | 0.00000 |
| 1084 | 107 | ARG | HH21 | -43.86541 |   | -44.15096 | 102.05452 | B1 | 25 | 0.00000 |

FIG. 18

00013077 013698

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|      |     |     |      |           |    |           |           |    |    |         |
|------|-----|-----|------|-----------|----|-----------|-----------|----|----|---------|
| 1085 | 107 | ARG | HH22 | -42.      | 04 | -45.11997 | 101.94496 | B1 | 25 | 0.00000 |
| 1086 | 107 | ARG | C    | -42.37787 |    | -41.03546 | 106.32504 | B1 | 25 | 0.00000 |
| 1087 | 107 | ARG | O    | -43.36896 |    | -40.31981 | 106.43645 | B1 | 25 | 0.00000 |
| 1088 | 108 | LEU | N    | -41.12633 |    | -40.58602 | 106.39627 | B1 | 26 | 0.00000 |
| 1089 | 108 | LEU | H    | -40.32617 |    | -41.17985 | 106.29320 | B1 | 26 | 0.00000 |
| 1090 | 108 | LEU | CA   | -40.89942 |    | -39.15744 | 106.53751 | B1 | 26 | 0.00000 |
| 1091 | 108 | LEU | CB   | -40.80087 |    | -38.80954 | 108.01248 | B1 | 26 | 0.00000 |
| 1092 | 108 | LEU | CG   | -41.96347 |    | -37.89689 | 108.35874 | B1 | 26 | 0.00000 |
| 1093 | 108 | LEU | CD1  | -42.75820 |    | -38.44729 | 109.53808 | B1 | 26 | 0.00000 |
| 1094 | 108 | LEU | CD2  | -41.50070 |    | -36.44650 | 108.50151 | B1 | 26 | 0.00000 |
| 1095 | 108 | LEU | C    | -39.62061 |    | -38.77273 | 105.85764 | B1 | 26 | 0.00000 |
| 1096 | 108 | LEU | O    | -38.76368 |    | -39.61093 | 105.60154 | B1 | 26 | 0.00000 |
| 1097 | 109 | LEU | N    | -39.52150 |    | -37.47828 | 105.56773 | B1 | 27 | 0.00000 |
| 1098 | 109 | LEU | H    | -40.28459 |    | -36.84167 | 105.72467 | B1 | 27 | 0.00000 |
| 1099 | 109 | LEU | CA   | -38.30683 |    | -37.02679 | 104.90334 | B1 | 27 | 0.00000 |
| 1100 | 109 | LEU | CB   | -38.47418 |    | -37.24039 | 103.39009 | B1 | 27 | 0.00000 |
| 1101 | 109 | LEU | CG   | -39.74490 |    | -36.59695 | 102.82634 | B1 | 27 | 0.00000 |
| 1102 | 109 | LEU | CD1  | -39.42210 |    | -35.25631 | 102.17066 | B1 | 27 | 0.00000 |
| 1103 | 109 | LEU | CD2  | -40.49190 |    | -37.56523 | 101.91138 | B1 | 27 | 0.00000 |
| 1104 | 109 | LEU | C    | -37.99969 |    | -35.58061 | 105.21268 | B1 | 27 | 0.00000 |
| 1105 | 109 | LEU | O    | -38.88411 |    | -34.77322 | 105.47943 | B1 | 27 | 0.00000 |
| 1106 | 110 | GLU | N    | -36.70092 |    | -35.29768 | 105.12126 | B1 | 28 | 0.00000 |
| 1107 | 110 | GLU | H    | -36.01498 |    | -36.01786 | 105.00992 | B1 | 28 | 0.00000 |
| 1108 | 110 | GLU | CA   | -36.20315 |    | -33.92985 | 105.08184 | B1 | 28 | 0.00000 |
| 1109 | 110 | GLU | CB   | -35.80577 |    | -33.47627 | 106.49578 | B1 | 28 | 0.00000 |
| 1110 | 110 | GLU | CG   | -35.32216 |    | -32.02210 | 106.60993 | B1 | 28 | 0.00000 |
| 1111 | 110 | GLU | CD   | -33.63608 |    | -31.67178 | 106.30413 | B1 | 28 | 0.00000 |
| 1112 | 110 | GLU | OE1  | -33.37957 |    | -30.74951 | 106.10521 | B1 | 28 | 0.00000 |
| 1113 | 110 | GLU | OE2  | -33.05671 |    | -32.85201 | 106.36491 | B1 | 28 | 0.00000 |
| 1114 | 110 | GLU | C    | -35.01026 |    | -33.94076 | 104.15500 | B1 | 28 | 0.00000 |
| 1115 | 110 | GLU | O    | -34.25577 |    | -34.90807 | 104.11585 | B1 | 28 | 0.00000 |
| 1116 | 111 | ARG | N    | -34.89439 |    | -32.86843 | 103.37222 | B1 | 29 | 0.00000 |
| 1117 | 111 | ARG | H    | -35.61365 |    | -32.16766 | 103.37387 | B1 | 29 | 0.00000 |
| 1118 | 111 | ARG | CA   | -33.75645 |    | -32.74903 | 102.46249 | B1 | 29 | 0.00000 |
| 1119 | 111 | ARG | CB   | -33.99004 |    | -33.60407 | 101.20352 | B1 | 29 | 0.00000 |
| 1120 | 111 | ARG | CG   | -35.45106 |    | -33.70037 | 100.75305 | B1 | 29 | 0.00000 |
| 1121 | 111 | ARG | CD   | -35.67880 |    | -34.83036 | 99.75174  | B1 | 29 | 0.00000 |
| 1122 | 111 | ARG | NE   | -37.09124 |    | -35.21147 | 99.72614  | B1 | 29 | 0.00000 |
| 1123 | 111 | ARG | HE   | -37.71860 |    | -34.61357 | 100.22757 | B1 | 29 | 0.00000 |
| 1124 | 111 | ARG | CZ   | -37.50098 |    | -36.32384 | 99.09789  | B1 | 29 | 0.00000 |
| 1125 | 111 | ARG | NH1  | -38.78116 |    | -36.68971 | 99.16119  | B1 | 29 | 0.00000 |
| 1126 | 111 | ARG | NH11 | -39.12269 |    | -37.49888 | 98.68276  | B1 | 29 | 0.00000 |
| 1127 | 111 | ARG | NH12 | -39.43712 |    | -36.16699 | 99.70940  | B1 | 29 | 0.00000 |
| 1128 | 111 | ARG | NH2  | -36.63391 |    | -37.06893 | 98.41518  | B1 | 29 | 0.00000 |
| 1129 | 111 | ARG | NH21 | -36.91501 |    | -37.90348 | 97.94325  | B1 | 29 | 0.00000 |
| 1130 | 111 | ARG | NH22 | -35.67503 |    | -36.78688 | 98.36264  | B1 | 29 | 0.00000 |
| 1131 | 111 | ARG | C    | -33.49135 |    | -31.31194 | 102.08170 | B1 | 29 | 0.00000 |
| 1132 | 111 | ARG | O    | -34.39395 |    | -30.54569 | 101.76699 | B1 | 29 | 0.00000 |
| 1133 | 112 | CYS | N    | -32.20568 |    | -30.97057 | 102.12414 | B1 | 30 | 0.00000 |
| 1134 | 112 | CYS | H    | -31.50733 |    | -31.64380 | 102.37455 | B1 | 30 | 0.00000 |
| 1135 | 112 | CYS | CA   | -31.80468 |    | -29.62360 | 101.73826 | B1 | 30 | 0.00000 |
| 1136 | 112 | CYS | CB   | -31.12874 |    | -28.92365 | 102.91930 | B1 | 30 | 0.00000 |
| 1137 | 112 | CYS | SG   | -30.70297 |    | -27.19555 | 102.57697 | B1 | 30 | 0.00000 |
| 1138 | 112 | CYS | C    | -30.87388 |    | -29.64998 | 100.54380 | B1 | 30 | 0.00000 |
| 1139 | 112 | CYS | O    | -29.97769 |    | -30.48052 | 100.40406 | B1 | 30 | 0.00000 |
| 1140 | 113 | ILE | N    | -31.15975 |    | -28.70696 | 99.65078  | B1 | 31 | 0.00000 |
| 1141 | 113 | ILE | H    | -31.84193 |    | -28.00116 | 99.86111  | B1 | 31 | 0.00000 |
| 1142 | 113 | ILE | CA   | -30.55305 |    | -28.70228 | 98.32464  | B1 | 31 | 0.00000 |
| 1143 | 113 | ILE | CB   | -31.56021 |    | -29.33526 | 97.30706  | B1 | 31 | 0.00000 |
| 1144 | 113 | ILE | CG2  | -33.00339 |    | -29.37434 | 97.82323  | B1 | 31 | 0.00000 |
| 1145 | 113 | ILE | CG1  | -31.52431 |    | -26.74164 | 95.89635  | B1 | 31 | 0.00000 |
| 1146 | 113 | ILE | CD   | -32.44047 |    | -29.50025 | 94.92272  | B1 | 31 | 0.00000 |
| 1147 | 113 | ILE | C    | -33.08576 |    | -27.29665 | 97.96536  | B1 | 31 | 0.00000 |
| 1148 | 113 | ILE | O    | -30.75333 |    | -24.25900 | 98.21317  | B1 | 31 | 0.00000 |

FIG. 19

|      |     |     |         |           |           |           |    |         |         |
|------|-----|-----|---------|-----------|-----------|-----------|----|---------|---------|
| 114  | TYR | N   | -28.110 | -27.25564 | 97.41665  | B1        | 32 | 0.00000 |         |
| 1150 | 114 | TYR | H       | -28.42570 | -28.10151 | 97.10297  | D1 | 32      | 0.00000 |
| 1151 | 114 | TYR | CA      | -28.22036 | -25.98264 | 97.11462  | B1 | 32      | 0.00000 |
| 1152 | 114 | TYR | CB      | -26.80088 | -26.01933 | 97.71345  | B1 | 32      | 0.00000 |
| 1153 | 114 | TYR | CG      | -26.01127 | -24.72107 | 97.61311  | B1 | 32      | 0.00000 |
| 1154 | 114 | TYR | CD1     | -26.62770 | -23.45825 | 97.79068  | B1 | 32      | 0.00000 |
| 1155 | 114 | TYR | CE1     | -25.84886 | -22.28083 | 97.75267  | B1 | 32      | 0.00000 |
| 1156 | 114 | TYR | CD2     | -24.61824 | -24.80211 | 97.38751  | B1 | 32      | 0.00000 |
| 1157 | 114 | TYR | CE2     | -23.83841 | -23.62651 | 97.34588  | B1 | 32      | 0.00000 |
| 1158 | 114 | TYR | CZ      | -24.45600 | -22.36940 | 97.53154  | B1 | 32      | 0.00000 |
| 1159 | 114 | TYR | OH      | -23.68967 | -21.21917 | 97.50979  | B1 | 32      | 0.00000 |
| 1160 | 114 | TYR | HH      | -22.79676 | -21.43015 | 97.21984  | B1 | 32      | 0.00000 |
| 1161 | 114 | TYR | C       | -28.14723 | -25.83215 | 95.61430  | B1 | 32      | 0.00000 |
| 1162 | 114 | TYR | O       | -27.66375 | -26.70965 | 94.91236  | B1 | 32      | 0.00000 |
| 1163 | 115 | ASN | N       | -28.66823 | -24.69995 | 95.12919  | B1 | 33      | 0.00000 |
| 1164 | 115 | ASN | H       | -29.03092 | -24.02391 | 95.77643  | B1 | 33      | 0.00000 |
| 1165 | 115 | ASN | CA      | -28.63762 | -24.41545 | 93.68566  | B1 | 33      | 0.00000 |
| 1166 | 115 | ASN | CB      | -27.27049 | -23.84385 | 93.27078  | B1 | 33      | 0.00000 |
| 1167 | 115 | ASN | CG      | -27.00239 | -22.43118 | 93.78440  | B1 | 33      | 0.00000 |
| 1168 | 115 | ASN | OD1     | -26.55389 | -22.16954 | 94.85370  | B1 | 33      | 0.00000 |
| 1169 | 115 | ASN | ND2     | -27.51765 | -21.48359 | 92.96271  | B1 | 33      | 0.00000 |
| 1170 | 115 | ASN | HD21    | -28.04883 | -21.70692 | 92.14797  | B1 | 33      | 0.00000 |
| 1171 | 115 | ASN | HD22    | -27.29503 | -20.52370 | 93.13946  | B1 | 33      | 0.00000 |
| 1172 | 115 | ASN | C       | -28.96318 | -25.59300 | 92.77321  | B1 | 33      | 0.00000 |
| 1173 | 115 | ASN | O       | -28.22150 | -25.91402 | 91.85250  | B1 | 33      | 0.00000 |
| 1174 | 116 | GLN | N       | -30.10651 | -26.23583 | 93.07767  | B1 | 34      | 0.00000 |
| 1175 | 116 | GLN | H       | -30.66790 | -25.52614 | 93.84830  | B1 | 34      | 0.00000 |
| 1176 | 116 | GLN | CA      | -30.60575 | -27.38897 | 92.31212  | B1 | 34      | 0.00000 |
| 1177 | 116 | GLN | CB      | -30.73906 | -26.98635 | 90.82631  | B1 | 34      | 0.00000 |
| 1178 | 116 | GLN | CG      | -31.33401 | -27.96419 | 89.80983  | B1 | 34      | 0.00000 |
| 1179 | 116 | GLN | CD      | -31.33954 | -27.31473 | 88.43508  | B1 | 34      | 0.00000 |
| 1180 | 116 | GLN | OE1     | -32.32002 | -27.33002 | 87.70605  | B1 | 34      | 0.00000 |
| 1181 | 116 | GLN | NE2     | -30.20428 | -26.71450 | 88.08185  | B1 | 34      | 0.00000 |
| 1182 | 116 | GLN | HE21    | -29.39553 | -26.71396 | 88.67007  | B1 | 34      | 0.00000 |
| 1183 | 116 | GLN | HE22    | -30.15594 | -26.24641 | 87.20205  | B1 | 34      | 0.00000 |
| 1184 | 116 | GLN | C       | -29.89899 | -28.73663 | 92.53043  | B1 | 34      | 0.00000 |
| 1185 | 116 | GLN | O       | -30.38571 | -29.77653 | 92.10767  | B1 | 34      | 0.00000 |
| 1186 | 117 | GLU | N       | -28.76921 | -28.72803 | 93.24838  | B1 | 35      | 0.00000 |
| 1187 | 117 | GLU | H       | -28.34990 | -27.88576 | 93.59525  | B1 | 35      | 0.00000 |
| 1188 | 117 | GLU | CA      | -28.17324 | -30.02538 | 93.58636  | B1 | 35      | 0.00000 |
| 1189 | 117 | GLU | CB      | -26.68237 | -30.02305 | 93.23572  | B1 | 35      | 0.00000 |
| 1190 | 117 | GLU | CG      | -26.41125 | -29.71932 | 91.75724  | B1 | 35      | 0.00000 |
| 1191 | 117 | GLU | CD      | -24.93459 | -29.87167 | 91.43636  | B1 | 35      | 0.00000 |
| 1192 | 117 | GLU | OE1     | -24.62388 | -30.40776 | 90.37359  | B1 | 35      | 0.00000 |
| 1193 | 117 | GLU | OE2     | -24.09945 | -29.45965 | 92.24135  | B1 | 35      | 0.00000 |
| 1194 | 117 | GLU | C       | -28.34342 | -30.35133 | 95.05360  | B1 | 35      | 0.00000 |
| 1195 | 117 | GLU | O       | -28.39032 | -29.54087 | 95.93593  | B1 | 35      | 0.00000 |
| 1196 | 118 | GLU | N       | -28.45418 | -31.70267 | 95.31151  | B1 | 36      | 0.00000 |
| 1197 | 118 | GLU | H       | -28.37884 | -32.37663 | 94.57056  | B1 | 36      | 0.00000 |
| 1198 | 118 | GLU | CA      | -20.64640 | -32.12718 | 96.70504  | B1 | 36      | 0.00000 |
| 1199 | 118 | GLU | CB      | -28.86529 | -33.64399 | 96.80220  | B1 | 36      | 0.00000 |
| 1200 | 118 | GLU | CG      | -30.04621 | -34.25904 | 96.04454  | B1 | 36      | 0.00000 |
| 1201 | 118 | GLU | CD      | -30.18685 | -35.73854 | 96.39969  | B1 | 36      | 0.00000 |
| 1202 | 118 | GLU | OE1     | -31.31366 | -36.18552 | 96.62004  | B1 | 36      | 0.00000 |
| 1203 | 118 | GLU | OE2     | -29.17775 | -36.44658 | 96.46236  | B1 | 36      | 0.00000 |
| 1204 | 118 | GLU | C       | -27.45968 | -31.79603 | 97.59954  | B1 | 36      | 0.00000 |
| 1205 | 118 | GLU | O       | -26.30375 | -31.93771 | 97.22004  | B1 | 36      | 0.00000 |
| 1206 | 119 | SER | N       | -27.77719 | -31.35385 | 98.81571  | B1 | 37      | 0.00000 |
| 1207 | 119 | SER | H       | -28.73032 | -31.22468 | 99.10568  | B1 | 37      | 0.00000 |
| 1208 | 119 | SER | CA      | -26.67523 | -31.09310 | 99.74333  | B1 | 37      | 0.00000 |
| 1209 | 119 | SER | CB      | -26.79679 | -29.64425 | 100.25438 | B1 | 37      | 0.00000 |
| 1210 | 119 | SER | CG      | -25.62406 | -29.23340 | 100.96654 | B1 | 37      | 0.00000 |
| 1211 | 119 | SER | HG      | -25.73840 | -28.33730 | 101.30354 | B1 | 37      | 0.00000 |
| 1212 | 119 | SER | C       | -26.64967 | -32.10859 | 100.87599 | B1 | 37      | 0.00000 |

FIG. 20

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|      |     |     |      |           |           |           |    |    |         |
|------|-----|-----|------|-----------|-----------|-----------|----|----|---------|
| 1213 | 119 | SER | O    | -25.7118  | -32.90554 | 101.03211 | B1 | 37 | 0.00000 |
| 1214 | 120 | VAL | N    | -27.72434 | -32.06608 | 101.67561 | B1 | 38 | 0.00000 |
| 1215 | 120 | VAL | H    | -28.50026 | -31.45938 | 101.48344 | B1 | 38 | 0.00000 |
| 1216 | 120 | VAL | CA   | -27.82678 | -32.99802 | 102.80099 | B1 | 38 | 0.00000 |
| 1217 | 120 | VAL | CB   | -27.44790 | -32.32244 | 104.13888 | B1 | 38 | 0.00000 |
| 1218 | 120 | VAL | CG1  | -25.93252 | -32.18078 | 104.29388 | B1 | 38 | 0.00000 |
| 1219 | 120 | VAL | CG2  | -28.15631 | -30.97900 | 104.33500 | B1 | 38 | 0.00000 |
| 1220 | 120 | VAL | C    | -29.23777 | -33.53625 | 102.89372 | B1 | 38 | 0.00000 |
| 1221 | 120 | VAL | O    | -30.19812 | -32.88656 | 102.49711 | B1 | 38 | 0.00000 |
| 1222 | 121 | ARG | N    | -29.34164 | -34.75356 | 103.41944 | B1 | 39 | 0.00000 |
| 1223 | 121 | ARG | H    | -28.52525 | -35.27675 | 103.67737 | B1 | 39 | 0.00000 |
| 1224 | 121 | ARG | CA   | -30.65941 | -35.37282 | 103.49447 | B1 | 39 | 0.00000 |
| 1225 | 121 | ARG | CB   | -30.83879 | -36.26556 | 102.25451 | B1 | 39 | 0.00000 |
| 1226 | 121 | ARG | CG   | -32.24891 | -36.83907 | 102.13977 | B1 | 39 | 0.00000 |
| 1227 | 121 | ARG | CD   | -32.36448 | -38.11228 | 101.31436 | B1 | 39 | 0.00000 |
| 1228 | 121 | ARG | NE   | -33.46636 | -38.89614 | 101.86585 | B1 | 39 | 0.00000 |
| 1229 | 121 | ARG | HE   | -33.58314 | -38.82444 | 102.86363 | B1 | 39 | 0.00000 |
| 1230 | 121 | ARG | CZ   | -34.21779 | -39.71705 | 101.13259 | B1 | 39 | 0.00000 |
| 1231 | 121 | ARG | NH1  | -35.18842 | -40.40193 | 101.73316 | B1 | 39 | 0.00000 |
| 1232 | 121 | ARG | NH11 | -35.77971 | -41.03741 | 101.23780 | B1 | 39 | 0.00000 |
| 1233 | 121 | ARG | NH12 | -35.33365 | -40.28453 | 102.71808 | B1 | 39 | 0.00000 |
| 1234 | 121 | ARG | NH2  | -33.99786 | -39.84536 | 99.82444  | B1 | 39 | 0.00000 |
| 1235 | 121 | ARG | NH21 | -34.53079 | -40.47140 | 99.25675  | B1 | 39 | 0.00000 |
| 1236 | 121 | ARG | NH22 | -33.27054 | -39.30635 | 99.39731  | B1 | 39 | 0.00000 |
| 1237 | 121 | ARG | C    | -30.80743 | -36.21013 | 104.75602 | B1 | 39 | 0.00000 |
| 1238 | 121 | ARG | O    | -29.86515 | -36.62872 | 105.23483 | B1 | 39 | 0.00000 |
| 1239 | 122 | PHE | N    | -32.04075 | -36.24055 | 105.26404 | B1 | 40 | 0.00000 |
| 1240 | 122 | PHE | H    | -32.75061 | -35.63810 | 104.89111 | B1 | 40 | 0.00000 |
| 1241 | 122 | PHE | CA   | -32.40668 | -37.26064 | 106.24769 | B1 | 40 | 0.00000 |
| 1242 | 122 | PHE | CB   | -33.75724 | -36.87165 | 106.85296 | B1 | 40 | 0.00000 |
| 1243 | 122 | PHE | CG   | -33.64992 | -36.46831 | 108.30418 | B1 | 40 | 0.00000 |
| 1244 | 122 | PHE | CD1  | -32.56100 | -35.69712 | 108.77664 | B1 | 40 | 0.00000 |
| 1245 | 122 | PHE | CD2  | -34.66985 | -36.87929 | 109.19094 | B1 | 40 | 0.00000 |
| 1246 | 122 | PHE | CE1  | -32.49275 | -35.34303 | 110.14035 | B1 | 40 | 0.00000 |
| 1247 | 122 | PHE | CE2  | -34.60187 | -36.52254 | 110.55431 | B1 | 40 | 0.00000 |
| 1248 | 122 | PHE | CZ   | -33.51285 | -35.75823 | 111.02379 | B1 | 40 | 0.00000 |
| 1249 | 122 | PHE | C    | -32.57844 | -38.62424 | 105.60697 | B1 | 40 | 0.00000 |
| 1250 | 122 | PHE | O    | -33.34168 | -38.79208 | 104.65587 | B1 | 40 | 0.00000 |
| 1251 | 123 | ASP | N    | -31.06201 | -39.60796 | 106.15389 | B1 | 41 | 0.00000 |
| 1252 | 123 | ASP | H    | -31.23184 | -39.47015 | 106.92548 | B1 | 41 | 0.00000 |
| 1253 | 123 | ASP | CA   | -32.08552 | -40.93522 | 105.58825 | B1 | 41 | 0.00000 |
| 1254 | 123 | ASP | CB   | -30.85171 | -41.81726 | 105.76445 | B1 | 41 | 0.00000 |
| 1255 | 123 | ASP | CG   | -29.93161 | -41.56041 | 104.59405 | B1 | 41 | 0.00000 |
| 1256 | 123 | ASP | OD1  | -28.81173 | -41.11310 | 104.81757 | B1 | 41 | 0.00000 |
| 1257 | 123 | ASP | OD2  | -30.34905 | -41.80191 | 103.45856 | B1 | 41 | 0.00000 |
| 1258 | 123 | ASP | C    | -33.32362 | -41.63618 | 106.09965 | B1 | 41 | 0.00000 |
| 1259 | 123 | ASP | O    | -34.00966 | -41.21121 | 107.02319 | B1 | 41 | 0.00000 |
| 1260 | 124 | SER | N    | -33.62443 | -42.74250 | 105.41429 | B1 | 42 | 0.00000 |
| 1261 | 124 | SER | H    | -32.95329 | -43.10971 | 104.76900 | B1 | 42 | 0.00000 |
| 1262 | 124 | SER | CA   | -34.94425 | -43.35498 | 105.58880 | B1 | 42 | 0.00000 |
| 1263 | 124 | SER | CB   | -35.18779 | -44.37028 | 104.46149 | B1 | 42 | 0.00000 |
| 1264 | 124 | SER | OG   | -36.57945 | -44.70776 | 104.37671 | B1 | 42 | 0.00000 |
| 1265 | 124 | SER | HG   | -36.91089 | -44.87590 | 105.27413 | B1 | 42 | 0.00000 |
| 1266 | 124 | SER | C    | -35.21640 | -44.01057 | 106.93634 | B1 | 42 | 0.00000 |
| 1267 | 124 | SER | O    | -36.33538 | -44.42223 | 107.22372 | B1 | 42 | 0.00000 |
| 1268 | 125 | ASP | N    | -34.16447 | -44.10325 | 107.74330 | B1 | 43 | 0.00000 |
| 1269 | 125 | ASP | H    | -33.26228 | -43.73425 | 107.50494 | B1 | 43 | 0.00000 |
| 1270 | 125 | ASP | CA   | -34.30492 | -44.60689 | 109.10471 | B1 | 43 | 0.00000 |
| 1271 | 125 | ASP | CB   | -32.96210 | -45.24580 | 109.50620 | B1 | 43 | 0.00000 |
| 1272 | 125 | ASP | CG   | -31.82155 | -44.23245 | 109.55779 | B1 | 43 | 0.00000 |
| 1273 | 125 | ASP | OD1  | -31.89194 | -43.19553 | 108.89075 | B1 | 43 | 0.00000 |
| 1274 | 125 | ASP | OD2  | -30.67249 | -44.45676 | 110.29614 | B1 | 43 | 0.00000 |
| 1275 | 125 | ASP | C    | -34.69374 | -43.52244 | 110.10428 | B1 | 43 | 0.00000 |
| 1276 | 125 | ASP | O    | -35.10540 | -43.76441 | 111.22672 | B1 | 43 | 0.00000 |

FIG. 21

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|      |     |     |      |           |           |           |    |    |         |
|------|-----|-----|------|-----------|-----------|-----------|----|----|---------|
| 1277 | 126 | VAL | N    | -34.51    | -42.26751 | 109.64790 | B1 | 44 | 0.00000 |
| 1278 | 126 | VAL | H    | -34.20939 | -42.12308 | 108.70456 | B1 | 44 | 0.00000 |
| 1279 | 126 | VAL | CA   | -34.59346 | -41.07914 | 110.50496 | B1 | 44 | 0.00000 |
| 1280 | 126 | VAL | CB   | -36.04814 | -40.82462 | 110.97592 | B1 | 44 | 0.00000 |
| 1281 | 126 | VAL | CG1  | -36.22164 | -39.41758 | 111.54094 | B1 | 44 | 0.00000 |
| 1282 | 126 | VAL | CG2  | -37.04494 | -41.00281 | 109.82481 | B1 | 44 | 0.00000 |
| 1283 | 126 | VAL | C    | -33.57625 | -41.13739 | 111.64961 | B1 | 44 | 0.00000 |
| 1284 | 126 | VAL | O    | -33.78819 | -40.75401 | 112.79533 | B1 | 44 | 0.00000 |
| 1285 | 127 | GLY | N    | -32.41541 | -41.66443 | 111.25324 | B1 | 45 | 0.00000 |
| 1286 | 127 | GLY | H    | -32.31598 | -42.01122 | 110.31755 | B1 | 45 | 0.00000 |
| 1287 | 127 | GLY | CA   | -31.32244 | -41.88201 | 112.19529 | B1 | 45 | 0.00000 |
| 1288 | 127 | GLY | C    | -29.94594 | -41.56889 | 111.62542 | B1 | 45 | 0.00000 |
| 1289 | 127 | GLY | O    | -29.03055 | -41.21776 | 112.35962 | B1 | 45 | 0.00000 |
| 1290 | 128 | GLU | N    | -29.81143 | -41.65704 | 110.29545 | B1 | 46 | 0.00000 |
| 1291 | 128 | GLU | H    | -30.48653 | -42.13586 | 109.72534 | B1 | 46 | 0.00000 |
| 1292 | 128 | GLU | CA   | -28.56256 | -41.14297 | 109.73120 | B1 | 46 | 0.00000 |
| 1293 | 128 | GLU | CB   | -27.75197 | -42.29481 | 109.11709 | B1 | 46 | 0.00000 |
| 1294 | 128 | GLU | CG   | -26.29316 | -42.25781 | 109.59860 | B1 | 46 | 0.00000 |
| 1295 | 128 | GLU | CD   | -25.44181 | -43.20422 | 108.87693 | B1 | 46 | 0.00000 |
| 1296 | 128 | GLU | OE1  | -24.49646 | -42.88073 | 108.19992 | B1 | 46 | 0.00000 |
| 1297 | 128 | GLU | OE2  | -25.71010 | -44.47773 | 109.00348 | B1 | 46 | 0.00000 |
| 1298 | 128 | GLU | C    | -28.71376 | -39.98012 | 108.75031 | B1 | 46 | 0.00000 |
| 1299 | 128 | GLU | O    | -29.80604 | -39.57375 | 108.35724 | B1 | 46 | 0.00000 |
| 1300 | 129 | TYR | N    | -27.54735 | -39.42619 | 108.38931 | B1 | 47 | 0.00000 |
| 1301 | 129 | TYR | H    | -26.68498 | -39.83420 | 108.68820 | B1 | 47 | 0.00000 |
| 1302 | 129 | TYR | CA   | -27.50019 | -38.29454 | 107.46434 | B1 | 47 | 0.00000 |
| 1303 | 129 | TYR | CB   | -26.63842 | -37.15326 | 108.01560 | B1 | 47 | 0.00000 |
| 1304 | 129 | TYR | CG   | -27.30857 | -36.34222 | 109.09443 | B1 | 47 | 0.00000 |
| 1305 | 129 | TYR | CD1  | -26.67181 | -36.21958 | 110.34811 | B1 | 47 | 0.00000 |
| 1306 | 129 | TYR | CE1  | -27.25566 | -35.42131 | 111.35148 | B1 | 47 | 0.00000 |
| 1307 | 129 | TYR | CD2  | -20.52827 | -35.67832 | 108.83210 | B1 | 47 | 0.00000 |
| 1308 | 129 | TYR | CE2  | -29.11235 | -34.88063 | 109.83571 | B1 | 47 | 0.00000 |
| 1309 | 129 | TYR | CZ   | -28.47327 | -34.75726 | 111.08860 | B1 | 47 | 0.00000 |
| 1310 | 129 | TYR | OH   | -29.05005 | -33.98459 | 112.07221 | B1 | 47 | 0.00000 |
| 1311 | 129 | TYR | HH   | -29.70394 | -33.40059 | 111.67732 | B1 | 47 | 0.00000 |
| 1312 | 129 | TYR | C    | -26.82531 | -38.64384 | 106.15941 | B1 | 47 | 0.00000 |
| 1313 | 129 | TYR | O    | -25.66697 | -39.04407 | 106.10492 | B1 | 47 | 0.00000 |
| 1314 | 130 | ARG | N    | -27.55686 | -38.38162 | 105.08581 | B1 | 48 | 0.00000 |
| 1315 | 130 | ARG | H    | -28.51666 | -38.10451 | 105.16735 | B1 | 48 | 0.00000 |
| 1316 | 130 | ARG | CA   | -26.07326 | -38.41254 | 103.80227 | B1 | 48 | 0.00000 |
| 1317 | 130 | ARG | CB   | -27.85650 | -38.64699 | 102.71647 | B1 | 48 | 0.00000 |
| 1318 | 130 | ARG | CG   | -27.21143 | -39.00526 | 101.34112 | B1 | 48 | 0.00000 |
| 1319 | 130 | ARG | CD   | -28.23975 | -39.41974 | 100.29808 | B1 | 48 | 0.00000 |
| 1320 | 130 | ARG | NE   | -27.66322 | -39.38333 | 98.95629  | B1 | 48 | 0.00000 |
| 1321 | 130 | ARG | HE   | -26.82589 | -38.85034 | 98.82833  | B1 | 48 | 0.00000 |
| 1322 | 130 | ARG | CZ   | -28.29934 | -39.96348 | 97.93202  | B1 | 48 | 0.00000 |
| 1323 | 130 | ARG | NH1  | -27.82365 | -39.81313 | 96.69917  | B1 | 48 | 0.00000 |
| 1324 | 130 | ARG | NH11 | -28.26738 | -40.23513 | 95.90996  | B1 | 48 | 0.00000 |
| 1325 | 130 | ARG | NH12 | -27.01064 | -39.25297 | 96.53955  | B1 | 48 | 0.00000 |
| 1326 | 130 | ARG | NH2  | -29.39843 | -40.68730 | 98.14392  | B1 | 48 | 0.00000 |
| 1327 | 130 | ARG | NH21 | -29.90446 | -41.10492 | 97.39118  | B1 | 48 | 0.00000 |
| 1328 | 130 | ARG | NH22 | -29.72741 | -40.81930 | 99.07957  | B1 | 48 | 0.00000 |
| 1329 | 130 | ARG | C    | -26.28084 | -37.06053 | 103.45986 | B1 | 48 | 0.00000 |
| 1330 | 130 | ARG | O    | -26.96293 | -36.11772 | 103.07688 | B1 | 48 | 0.00000 |
| 1331 | 131 | ALA | N    | -24.95816 | -36.99899 | 103.58668 | B1 | 49 | 0.00000 |
| 1332 | 131 | ALA | H    | -24.45069 | -37.77908 | 103.95192 | B1 | 49 | 0.00000 |
| 1333 | 131 | ALA | CA   | -24.28607 | -35.84094 | 102.98902 | B1 | 49 | 0.00000 |
| 1334 | 131 | ALA | CB   | -23.06137 | -35.44271 | 103.80801 | B1 | 49 | 0.00000 |
| 1335 | 131 | ALA | C    | -23.85084 | -36.20633 | 101.58658 | B1 | 49 | 0.00000 |
| 1336 | 131 | ALA | O    | -23.17892 | -37.20652 | 101.36065 | B1 | 49 | 0.00000 |
| 1337 | 132 | VAL | N    | -24.28495 | -35.38774 | 100.63154 | B1 | 50 | 0.00000 |
| 1338 | 132 | VAL | H    | -24.78984 | -34.54695 | 100.25567 | B1 | 50 | 0.00000 |
| 1339 | 132 | VAL | CA   | -24.05920 | -35.79619 | 99.24152  | B1 | 50 | 0.00000 |
| 1340 | 132 | VAL | CB   | -25.12578 | -35.11200 | 99.36560  | B1 | 50 | 0.00000 |

FIG. 22

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22

|      |     |     |      |           |           |           |    |    |         |
|------|-----|-----|------|-----------|-----------|-----------|----|----|---------|
| 1341 | 132 | VAL | CG1  | -25.05    | -35.45687 | 96.87606  | B1 | 50 | 0.00000 |
| 1342 | 132 | VAL | CG2  | -26.51048 | -35.48853 | 98.85777  | B1 | 50 | 0.00000 |
| 1343 | 132 | VAL | C    | -22.64446 | -35.53393 | 98.73419  | B1 | 50 | 0.00000 |
| 1344 | 132 | VAL | O    | -22.12598 | -36.19257 | 97.84114  | B1 | 50 | 0.00000 |
| 1345 | 133 | THR | N    | -22.01646 | -34.53567 | 99.35299  | B1 | 51 | 0.00000 |
| 1346 | 133 | THR | H    | -22.44036 | -34.04272 | 100.11190 | B1 | 51 | 0.00000 |
| 1347 | 133 | THR | CA   | -20.68297 | -34.13851 | 98.91128  | B1 | 51 | 0.00000 |
| 1348 | 133 | THR | CB   | -20.84979 | -33.09962 | 97.76600  | B1 | 51 | 0.00000 |
| 1349 | 133 | THR | OG1  | -19.58519 | -32.56706 | 97.34397  | B1 | 51 | 0.00000 |
| 1350 | 133 | THR | HG1  | -19.69018 | -32.10136 | 96.50551  | B1 | 51 | 0.00000 |
| 1351 | 133 | THR | CG2  | -21.81730 | -31.96947 | 98.12788  | B1 | 51 | 0.00000 |
| 1352 | 133 | THR | C    | -19.91735 | -33.59750 | 100.10846 | B1 | 51 | 0.00000 |
| 1353 | 133 | THR | O    | -20.48697 | -33.30952 | 101.15881 | B1 | 51 | 0.00000 |
| 1354 | 134 | GLU | N    | -18.60119 | -33.44216 | 99.91793  | B1 | 52 | 0.00000 |
| 1355 | 134 | GLU | H    | -18.20352 | -33.65725 | 99.02398  | B1 | 52 | 0.00000 |
| 1356 | 134 | GLU | CA   | -17.75238 | -32.88738 | 100.97647 | B1 | 52 | 0.00000 |
| 1357 | 134 | GLU | CB   | -16.30452 | -32.81284 | 100.49482 | B1 | 52 | 0.00000 |
| 1358 | 134 | GLU | CG   | -15.76229 | -34.17073 | 100.03844 | B1 | 52 | 0.00000 |
| 1359 | 134 | GLU | CD   | -14.31377 | -34.04410 | 99.60488  | B1 | 52 | 0.00000 |
| 1360 | 134 | GLU | OE1  | -13.54341 | -34.96158 | 99.88007  | B1 | 52 | 0.00000 |
| 1361 | 134 | GLU | OE2  | -13.96021 | -33.03519 | 98.99487  | B1 | 52 | 0.00000 |
| 1362 | 134 | GLU | C    | -18.18601 | -31.51310 | 101.45728 | B1 | 52 | 0.00000 |
| 1363 | 134 | GLU | O    | -17.97884 | -31.11916 | 102.59352 | B1 | 52 | 0.00000 |
| 1364 | 135 | LEU | N    | -18.87611 | -30.80674 | 100.55812 | B1 | 53 | 0.00000 |
| 1365 | 135 | LEU | H    | -18.92762 | -31.13340 | 99.61398  | B1 | 53 | 0.00000 |
| 1366 | 135 | LEU | CA   | -19.55727 | -29.57029 | 100.94521 | B1 | 53 | 0.00000 |
| 1367 | 135 | LEU | CB   | -20.25914 | -29.06218 | 99.70959  | B1 | 53 | 0.00000 |
| 1368 | 135 | LEU | CG   | -20.12211 | -27.57937 | 99.38843  | B1 | 53 | 0.00000 |
| 1369 | 135 | LEU | CD1  | -20.93390 | -26.68772 | 100.32666 | B1 | 53 | 0.00000 |
| 1370 | 135 | LEU | CD2  | -18.63204 | -27.23870 | 99.36436  | B1 | 53 | 0.00000 |
| 1371 | 135 | LEU | C    | -20.53099 | -29.72915 | 102.11412 | B1 | 53 | 0.00000 |
| 1372 | 135 | LEU | O    | -20.60025 | -28.93514 | 103.04463 | B1 | 53 | 0.00000 |
| 1373 | 136 | GLY | N    | -21.29082 | -30.82221 | 102.02891 | B1 | 54 | 0.00000 |
| 1374 | 136 | GLY | H    | -21.14062 | -31.49656 | 101.30480 | B1 | 54 | 0.00000 |
| 1375 | 136 | GLY | CA   | -22.25373 | -31.10000 | 103.08935 | B1 | 54 | 0.00000 |
| 1376 | 136 | GLY | C    | -21.66227 | -31.85099 | 104.26834 | B1 | 54 | 0.00000 |
| 1377 | 136 | GLY | O    | -22.17280 | -31.82013 | 105.38053 | B1 | 54 | 0.00000 |
| 1378 | 137 | ARG | N    | -20.54192 | -32.53644 | 104.01306 | B1 | 55 | 0.00000 |
| 1379 | 137 | ARG | H    | -20.17033 | -32.57514 | 103.08296 | B1 | 55 | 0.00000 |
| 1380 | 137 | ARG | CA   | -19.94165 | -33.32437 | 105.09532 | B1 | 55 | 0.00000 |
| 1381 | 137 | ARG | CB   | -18.67070 | -34.02762 | 104.58318 | B1 | 55 | 0.00000 |
| 1382 | 137 | ARG | CG   | -18.13008 | -35.07893 | 105.55025 | B1 | 55 | 0.00000 |
| 1383 | 137 | ARG | CD   | -19.16855 | -36.15719 | 105.85371 | B1 | 55 | 0.00000 |
| 1384 | 137 | ARG | NE   | -18.66781 | -37.06640 | 106.87657 | B1 | 55 | 0.00000 |
| 1385 | 137 | ARG | HE   | -17.93002 | -36.71980 | 107.47204 | B1 | 55 | 0.00000 |
| 1386 | 137 | ARG | CZ   | -19.21896 | -38.26612 | 107.07006 | B1 | 55 | 0.00000 |
| 1387 | 137 | ARG | NH1  | -18.67534 | -39.07643 | 107.97489 | B1 | 55 | 0.00000 |
| 1388 | 137 | ARG | NH11 | -19.03969 | -39.99255 | 108.14749 | B1 | 55 | 0.00000 |
| 1389 | 137 | ARG | NH12 | -17.88763 | -38.75541 | 108.49972 | B1 | 55 | 0.00000 |
| 1390 | 137 | ARG | NH2  | -20.29085 | -38.64369 | 106.37214 | B1 | 55 | 0.00000 |
| 1391 | 137 | ARG | NH21 | -20.72192 | -39.53705 | 106.49834 | B1 | 55 | 0.00000 |
| 1392 | 137 | ARG | NH22 | -20.68879 | -38.01490 | 105.70437 | B1 | 55 | 0.00000 |
| 1393 | 137 | ARG | C    | -19.76330 | -32.65026 | 106.46929 | B1 | 55 | 0.00000 |
| 1394 | 137 | ARG | O    | -20.33202 | -33.13638 | 107.44172 | B1 | 55 | 0.00000 |
| 1395 | 138 | PRO | N    | -19.03095 | -31.51331 | 106.56277 | B1 | 56 | 0.00000 |
| 1396 | 138 | PRO | CD   | -18.26903 | -30.78028 | 105.55482 | B1 | 56 | 0.00000 |
| 1397 | 138 | PRO | CA   | -10.92500 | -30.86885 | 107.67839 | B1 | 56 | 0.00000 |
| 1398 | 138 | PRO | CB   | -18.00966 | -29.66775 | 107.61416 | B1 | 56 | 0.00000 |
| 1399 | 138 | PRO | CG   | -17.22521 | -30.01427 | 106.35369 | B1 | 56 | 0.00000 |
| 1400 | 138 | PRO | C    | -20.24853 | -30.39451 | 108.45452 | B1 | 56 | 0.00000 |
| 1401 | 138 | PRO | O    | -20.38673 | -30.20105 | 109.65243 | B1 | 56 | 0.00000 |
| 1402 | 139 | ASP | N    | -21.22622 | -30.19407 | 107.56513 | B1 | 57 | 0.00000 |
| 1403 | 139 | ASP | H    | -21.12955 | -30.45258 | 106.60295 | B1 | 57 | 0.00000 |
| 1404 | 139 | ASP | CA   | -22.54445 | -29.76374 | 108.02615 | B1 | 57 | 0.00000 |

FIG. 23

|      |     |     |      |           |   |           |           |    |    |         |
|------|-----|-----|------|-----------|---|-----------|-----------|----|----|---------|
| 1405 | 139 | ASP | CB   | -23.2     | 1 | -29.22794 | 106.80729 | B1 | 57 | 0.00000 |
| 1406 | 139 | ASP | CG   | -24.50000 |   | -28.44150 | 107.23406 | B1 | 57 | 0.00000 |
| 1407 | 139 | ASP | OD1  | -24.33925 |   | -27.25955 | 107.53698 | B1 | 57 | 0.00000 |
| 1408 | 139 | ASP | OD2  | -25.59590 |   | -29.00937 | 107.24891 | B1 | 57 | 0.00000 |
| 1409 | 139 | ASP | C    | -23.29009 |   | -30.90651 | 108.70646 | B1 | 57 | 0.00000 |
| 1410 | 139 | ASP | O    | -23.84428 |   | -30.79944 | 109.79628 | B1 | 57 | 0.00000 |
| 1411 | 140 | ALA | N    | -23.18867 |   | -32.06950 | 108.04975 | B1 | 58 | 0.00000 |
| 1412 | 140 | ALA | H    | -22.77745 |   | -32.09325 | 107.13514 | B1 | 58 | 0.00000 |
| 1413 | 140 | ALA | CA   | -23.64141 |   | -33.29863 | 108.70194 | B1 | 58 | 0.00000 |
| 1414 | 140 | ALA | CB   | -23.39932 |   | -34.51285 | 107.80148 | B1 | 58 | 0.00000 |
| 1415 | 140 | ALA | C    | -22.96994 |   | -33.52591 | 110.04660 | B1 | 58 | 0.00000 |
| 1416 | 140 | ALA | O    | -23.61501 |   | -33.62460 | 111.08086 | B1 | 58 | 0.00000 |
| 1417 | 141 | GLU | N    | -21.63141 |   | -33.53710 | 110.01537 | B1 | 59 | 0.00000 |
| 1418 | 141 | GLU | H    | -21.14260 |   | -33.44422 | 109.14251 | B1 | 59 | 0.00000 |
| 1419 | 141 | GLU | CA   | -20.88131 |   | -33.73045 | 111.26272 | B1 | 59 | 0.00000 |
| 1420 | 141 | GLU | CB   | -19.38545 |   | -33.75474 | 110.92637 | B1 | 59 | 0.00000 |
| 1421 | 141 | GLU | CG   | -19.08157 |   | -34.92155 | 109.97183 | B1 | 59 | 0.00000 |
| 1422 | 141 | GLU | CD   | -17.65605 |   | -34.91070 | 109.44677 | B1 | 59 | 0.00000 |
| 1423 | 141 | GLU | OE1  | -17.21662 |   | -35.95752 | 108.96182 | B1 | 59 | 0.00000 |
| 1424 | 141 | GLU | OE2  | -16.99658 |   | -33.87375 | 109.50268 | B1 | 59 | 0.00000 |
| 1425 | 141 | GLU | C    | -21.20315 |   | -32.72395 | 112.36696 | B1 | 59 | 0.00000 |
| 1426 | 141 | GLU | O    | -21.35204 |   | -33.05368 | 113.53869 | B1 | 59 | 0.00000 |
| 1427 | 142 | TYR | N    | -21.39109 |   | -31.47026 | 111.93865 | B1 | 60 | 0.00000 |
| 1428 | 142 | TYR | H    | -21.16858 |   | -31.22939 | 110.99159 | B1 | 60 | 0.00000 |
| 1429 | 142 | TYR | CA   | -21.91640 |   | -30.42572 | 112.82625 | B1 | 60 | 0.00000 |
| 1430 | 142 | TYR | CB   | -22.17510 |   | -29.18770 | 111.95478 | B1 | 60 | 0.00000 |
| 1431 | 142 | TYR | CG   | -22.15441 |   | -27.86866 | 112.68902 | B1 | 60 | 0.00000 |
| 1432 | 142 | TYR | CD1  | -20.91930 |   | -27.21121 | 112.86286 | B1 | 60 | 0.00000 |
| 1433 | 142 | TYR | CE1  | -20.89216 |   | -25.94177 | 113.49633 | B1 | 60 | 0.00000 |
| 1434 | 142 | TYR | CD2  | -23.36373 |   | -27.27306 | 113.11310 | B1 | 60 | 0.00000 |
| 1435 | 142 | TYR | CE2  | -23.33600 |   | -26.00211 | 113.72688 | B1 | 60 | 0.00000 |
| 1436 | 142 | TYR | CZ   | -22.10013 |   | -25.34007 | 113.91274 | B1 | 60 | 0.00000 |
| 1437 | 142 | TYR | OH   | -22.06472 |   | -24.08718 | 114.49226 | B1 | 60 | 0.00000 |
| 1438 | 142 | TYR | HH   | -22.95958 |   | -23.75980 | 114.62492 | B1 | 60 | 0.00000 |
| 1439 | 142 | TYR | C    | -23.20365 |   | -30.84932 | 113.52485 | B1 | 60 | 0.00000 |
| 1440 | 142 | TYR | O    | -23.33185 |   | -30.86335 | 114.74427 | B1 | 60 | 0.00000 |
| 1441 | 143 | TRP | N    | -24.16619 |   | -31.24530 | 112.69102 | B1 | 61 | 0.00000 |
| 1442 | 143 | TRP | H    | -24.01203 |   | -31.27353 | 111.69669 | B1 | 61 | 0.00000 |
| 1443 | 143 | TRP | CA   | -25.46084 |   | -31.65772 | 113.24427 | B1 | 61 | 0.00000 |
| 1444 | 143 | TRP | CB   | -26.46502 |   | -31.82534 | 112.10045 | B1 | 61 | 0.00000 |
| 1445 | 143 | TRP | CG   | -26.82927 |   | -30.51319 | 111.43167 | B1 | 61 | 0.00000 |
| 1446 | 143 | TRP | CD2  | -27.59514 |   | -30.35383 | 110.26190 | B1 | 61 | 0.00000 |
| 1447 | 143 | TRP | CE2  | -27.68725 |   | -28.88192 | 110.01923 | B1 | 61 | 0.00000 |
| 1448 | 143 | TRP | CE3  | -28.23171 |   | -31.24445 | 109.37526 | B1 | 61 | 0.00000 |
| 1449 | 143 | TRP | CD1  | -26.49404 |   | -29.20408 | 111.84528 | B1 | 61 | 0.00000 |
| 1450 | 143 | TRP | NE1  | -26.99373 |   | -28.24161 | 111.01939 | B1 | 61 | 0.00000 |
| 1451 | 143 | TRP | HE1  | -26.86335 |   | -27.27405 | 111.09738 | B1 | 61 | 0.00000 |
| 1452 | 143 | TRP | CZ2  | -28.41151 |   | -28.41903 | 108.90296 | B1 | 61 | 0.00000 |
| 1453 | 143 | TRP | CZ3  | -28.94655 |   | -30.73482 | 108.27056 | B1 | 61 | 0.00000 |
| 1454 | 143 | TRP | CH2  | -29.03488 |   | -29.34388 | 108.03833 | B1 | 61 | 0.00000 |
| 1455 | 143 | TRP | C    | -25.40824 |   | -32.93379 | 114.07770 | B1 | 61 | 0.00000 |
| 1456 | 143 | TRP | O    | -26.13451 |   | -33.11650 | 115.04995 | B1 | 61 | 0.00000 |
| 1457 | 144 | ASN | N    | -24.46546 |   | -33.80055 | 113.69236 | B1 | 62 | 0.00000 |
| 1458 | 144 | ASN | H    | -23.94027 |   | -33.62305 | 112.85783 | B1 | 62 | 0.00000 |
| 1459 | 144 | ASN | CA   | -24.16067 |   | -34.99080 | 114.49069 | B1 | 62 | 0.00000 |
| 1460 | 144 | ASN | CB   | -23.20850 |   | -35.93308 | 113.73882 | B1 | 62 | 0.00000 |
| 1461 | 144 | ASN | CG   | -23.89541 |   | -36.68861 | 112.61740 | B1 | 62 | 0.00000 |
| 1462 | 144 | ASN | OD1  | -23.68155 |   | -36.47075 | 111.43371 | B1 | 62 | 0.00000 |
| 1463 | 144 | ASN | ND2  | -24.72776 |   | -37.64097 | 113.02365 | B1 | 62 | 0.00000 |
| 1464 | 144 | ASN | HD21 | -24.69338 |   | -37.81526 | 113.99276 | B1 | 62 | 0.00000 |
| 1465 | 144 | ASN | HD22 | -25.19584 |   | -38.20406 | 112.34455 | B1 | 62 | 0.00000 |
| 1466 | 144 | ASN | C    | -23.49875 |   | -34.69497 | 115.82591 | B1 | 62 | 0.00000 |
| 1467 | 144 | ASN | O    | -23.43003 |   | -35.54654 | 116.69914 | B1 | 62 | 0.00000 |
| 1468 | 145 | SER | N    | -22.99604 |   | -33.46640 | 115.97315 | B1 | 63 | 0.00000 |

FIG. 24

00013077.012698



00013077 012698

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24

|      |     |     |      |           |    |           |           |    |    |         |
|------|-----|-----|------|-----------|----|-----------|-----------|----|----|---------|
| 1469 | 145 | SER | H    | -22.1     | 10 | -32.80428 | 115.21961 | B1 | 63 | 0.00000 |
| 1470 | 145 | SER | CA   | -22.35004 |    | -33.14621 | 117.25865 | B1 | 63 | 0.00000 |
| 1471 | 145 | SER | CB   | -20.91921 |    | -32.73054 | 117.01176 | B1 | 63 | 0.00000 |
| 1472 | 145 | SER | OG   | -20.18983 |    | -32.64180 | 118.24511 | B1 | 63 | 0.00000 |
| 1473 | 145 | SER | HG   | -20.76055 |    | -32.22535 | 118.91065 | B1 | 63 | 0.00000 |
| 1474 | 145 | SER | C    | -23.11027 |    | -32.07614 | 118.06161 | B1 | 63 | 0.00000 |
| 1475 | 145 | SER | O    | -22.67401 |    | -31.68287 | 119.13941 | B1 | 63 | 0.00000 |
| 1476 | 146 | GLN | N    | -24.22180 |    | -31.59037 | 117.51252 | B1 | 64 | 0.00000 |
| 1477 | 146 | GLN | H    | -24.58118 |    | -31.94604 | 116.64774 | B1 | 64 | 0.00000 |
| 1478 | 146 | GLN | CA   | -24.90025 |    | -30.49286 | 118.19522 | B1 | 64 | 0.00000 |
| 1479 | 146 | GLN | CB   | -24.86315 |    | -29.29301 | 117.23892 | B1 | 64 | 0.00000 |
| 1480 | 146 | GLN | CG   | -25.45855 |    | -27.96945 | 117.72882 | B1 | 64 | 0.00000 |
| 1481 | 146 | GLN | CD   | -26.89096 |    | -27.81462 | 117.25234 | B1 | 64 | 0.00000 |
| 1482 | 146 | GLN | OE1  | -27.00837 |    | -27.53609 | 118.00911 | B1 | 64 | 0.00000 |
| 1483 | 146 | GLN | NE2  | -27.06556 |    | -27.97948 | 115.94329 | B1 | 64 | 0.00000 |
| 1484 | 146 | GLN | HE21 | -26.30809 |    | -28.20349 | 115.33276 | B1 | 64 | 0.00000 |
| 1485 | 146 | GLN | HE22 | -27.98288 |    | -27.88997 | 115.56134 | B1 | 64 | 0.00000 |
| 1486 | 146 | GLN | C    | -26.29488 |    | -30.93694 | 118.57642 | B1 | 64 | 0.00000 |
| 1487 | 146 | GLN | O    | -27.21649 |    | -30.91839 | 117.77294 | B1 | 64 | 0.00000 |
| 1488 | 147 | LYS | N    | -26.36947 |    | -31.44426 | 119.82371 | B1 | 65 | 0.00000 |
| 1489 | 147 | LYS | H    | -25.65249 |    | -31.20699 | 120.47663 | B1 | 65 | 0.00000 |
| 1490 | 147 | LYS | CA   | -27.35463 |    | -32.46614 | 120.21964 | B1 | 65 | 0.00000 |
| 1491 | 147 | LYS | CB   | -28.27258 |    | -32.00851 | 121.37895 | B1 | 65 | 0.00000 |
| 1492 | 147 | LYS | CG   | -29.34716 |    | -33.02726 | 121.84203 | B1 | 65 | 0.00000 |
| 1493 | 147 | LYS | CD   | -28.88674 |    | -34.49172 | 121.97244 | B1 | 65 | 0.00000 |
| 1494 | 147 | LYS | CE   | -29.96618 |    | -35.46785 | 121.47444 | B1 | 65 | 0.00000 |
| 1495 | 147 | LYS | NZ   | -29.40221 |    | -36.81034 | 121.26907 | B1 | 65 | 0.00000 |
| 1496 | 147 | LYS | HZ1  | -30.04886 |    | -37.42223 | 120.71767 | B1 | 65 | 0.00000 |
| 1497 | 147 | LYS | HZ2  | -28.53282 |    | -36.76558 | 120.68922 | B1 | 65 | 0.00000 |
| 1498 | 147 | LYS | HZ3  | -29.15199 |    | -37.28892 | 122.15073 | B1 | 65 | 0.00000 |
| 1499 | 147 | LYS | C    | -28.12445 |    | -33.12689 | 119.09340 | B1 | 65 | 0.00000 |
| 1500 | 147 | LYS | O    | -29.30235 |    | -32.90174 | 118.83883 | B1 | 65 | 0.00000 |
| 1501 | 148 | ASP | N    | -27.34620 |    | -34.00916 | 118.45822 | B1 | 66 | 0.00000 |
| 1502 | 148 | ASP | H    | -26.39747 |    | -34.14495 | 118.75300 | B1 | 66 | 0.00000 |
| 1503 | 148 | ASP | CA   | -27.79510 |    | -35.00236 | 117.48362 | B1 | 66 | 0.00000 |
| 1504 | 148 | ASP | CB   | -27.88927 |    | -36.37833 | 118.17059 | B1 | 66 | 0.00000 |
| 1505 | 148 | ASP | CG   | -26.79528 |    | -36.57930 | 119.21585 | B1 | 66 | 0.00000 |
| 1506 | 148 | ASP | OD1  | -25.69280 |    | -36.06325 | 119.05193 | B1 | 66 | 0.00000 |
| 1507 | 148 | ASP | OD2  | -27.07650 |    | -37.20742 | 120.23524 | B1 | 66 | 0.00000 |
| 1508 | 148 | ASP | C    | -29.08887 |    | -34.63043 | 116.79645 | B1 | 66 | 0.00000 |
| 1509 | 148 | ASP | O    | -30.17136 |    | -35.14808 | 117.04951 | B1 | 66 | 0.00000 |
| 1510 | 149 | LEU | N    | -28.92399 |    | -33.61840 | 115.93941 | B1 | 67 | 0.00000 |
| 1511 | 149 | LEU | H    | -27.98965 |    | -33.30949 | 115.73440 | B1 | 67 | 0.00000 |
| 1512 | 149 | LEU | CA   | -30.07076 |    | -32.84036 | 115.45008 | B1 | 67 | 0.00000 |
| 1513 | 149 | LEU | CB   | -29.45399 |    | -31.74267 | 114.57360 | B1 | 67 | 0.00000 |
| 1514 | 149 | LEU | CG   | -30.29432 |    | -30.58223 | 114.02475 | B1 | 67 | 0.00000 |
| 1515 | 149 | LEU | CD1  | -30.85820 |    | -30.92475 | 112.65290 | B1 | 67 | 0.00000 |
| 1516 | 149 | LEU | CD2  | -31.34761 |    | -30.09615 | 115.02072 | B1 | 67 | 0.00000 |
| 1517 | 149 | LEU | C    | -31.17667 |    | -33.69413 | 114.80952 | B1 | 67 | 0.00000 |
| 1518 | 149 | LEU | O    | -32.36472 |    | -33.37859 | 114.83807 | B1 | 67 | 0.00000 |
| 1519 | 150 | LEU | N    | -30.73118 |    | -34.86138 | 114.32363 | B1 | 68 | 0.00000 |
| 1520 | 150 | LEU | H    | -29.75579 |    | -34.94139 | 114.11621 | B1 | 68 | 0.00000 |
| 1521 | 150 | LEU | CA   | -31.59782 |    | -36.02822 | 114.12850 | B1 | 68 | 0.00000 |
| 1522 | 150 | LEU | CB   | -30.74740 |    | -37.29867 | 114.15286 | B1 | 68 | 0.00000 |
| 1523 | 150 | LEU | CG   | -29.89363 |    | -37.44772 | 112.89569 | B1 | 68 | 0.00000 |
| 1524 | 150 | LEU | CD1  | -20.64060 |    | -38.26626 | 113.18796 | B1 | 68 | 0.00000 |
| 1525 | 150 | LEU | CD2  | -30.71709 |    | -38.01712 | 111.73915 | B1 | 68 | 0.00000 |
| 1526 | 150 | LEU | C    | -32.74973 |    | -36.17247 | 115.10785 | B1 | 68 | 0.00000 |
| 1527 | 150 | LEU | O    | -33.89001 |    | -36.01901 | 114.70350 | B1 | 68 | 0.00000 |
| 1528 | 151 | GLU | N    | -32.47441 |    | -36.43576 | 116.39428 | B1 | 69 | 0.00000 |
| 1529 | 151 | GLU | H    | -31.52943 |    | -36.57284 | 116.72119 | B1 | 69 | 0.00000 |
| 1530 | 151 | GLU | CA   | -33.61295 |    | -36.59512 | 117.30950 | B1 | 69 | 0.00000 |
| 1531 | 151 | GLU | CB   | -33.19469 |    | -36.98331 | 118.72928 | B1 | 69 | 0.00000 |
| 1532 | 151 | GLU | CG   | -32.69081 |    | -38.41906 | 118.86124 | B1 | 69 | 0.00000 |

FIG. 25

|      |     |     |      |           |           |           |    |    |         |
|------|-----|-----|------|-----------|-----------|-----------|----|----|---------|
| 1532 | 151 | GLU | CD   | -31.15287 | -38.44464 | 118.70497 | B1 | 69 | 0.00000 |
| 1534 | 151 | GLU | OE1  | -30.71320 | -30.33129 | 117.58148 | B1 | 69 | 0.00000 |
| 1535 | 151 | GLU | OE2  | -30.51522 | -38.56462 | 119.72459 | B1 | 69 | 0.00000 |
| 1536 | 151 | GLU | C    | -34.55067 | -35.41168 | 117.43857 | B1 | 69 | 0.00000 |
| 1537 | 151 | GLU | O    | -35.75790 | -35.57313 | 117.58647 | B1 | 69 | 0.00000 |
| 1538 | 152 | GLN | N    | -33.98601 | -34.19700 | 117.35586 | B1 | 70 | 0.00000 |
| 1539 | 152 | GLN | H    | -33.00321 | -34.10256 | 117.18602 | B1 | 70 | 0.00000 |
| 1540 | 152 | GLN | CA   | -34.89656 | -33.04752 | 117.40695 | B1 | 70 | 0.00000 |
| 1541 | 152 | GLN | CB   | -34.15680 | -31.71646 | 117.32018 | B1 | 70 | 0.00000 |
| 1542 | 152 | GLN | CG   | -33.46159 | -31.26900 | 118.60094 | B1 | 70 | 0.00000 |
| 1543 | 152 | GLN | CD   | -33.23376 | -29.77424 | 118.49387 | B1 | 70 | 0.00000 |
| 1544 | 152 | GLN | OE1  | -32.13068 | -29.27019 | 118.36008 | B1 | 70 | 0.00000 |
| 1545 | 152 | GLN | NE2  | -34.34656 | -29.04682 | 118.54711 | B1 | 70 | 0.00000 |
| 1546 | 152 | GLN | HE21 | -35.24607 | -29.46511 | 118.65663 | B1 | 70 | 0.00000 |
| 1547 | 152 | GLN | HE22 | -34.28188 | -28.05358 | 118.46911 | B1 | 70 | 0.00000 |
| 1548 | 152 | GLN | C    | -35.89575 | -33.04746 | 116.27182 | B1 | 70 | 0.00000 |
| 1549 | 152 | GLN | O    | -37.09756 | -32.85841 | 116.43607 | B1 | 70 | 0.00000 |
| 1550 | 153 | ARG | N    | -35.34435 | -33.30759 | 115.08552 | B1 | 71 | 0.00000 |
| 1551 | 153 | ARG | H    | -34.35839 | -33.48709 | 114.99299 | B1 | 71 | 0.00000 |
| 1552 | 153 | ARG | CA   | -36.25853 | -33.42129 | 119.95947 | B1 | 71 | 0.00000 |
| 1553 | 153 | ARG | CD   | -35.46322 | -33.43707 | 112.66564 | B1 | 71 | 0.00000 |
| 1554 | 153 | ARG | CG   | -34.84280 | -32.07791 | 112.35054 | B1 | 71 | 0.00000 |
| 1555 | 153 | ARG | CD   | -33.88499 | -32.22570 | 111.17839 | B1 | 71 | 0.00000 |
| 1556 | 153 | ARG | NE   | -33.53171 | -30.95306 | 110.55166 | B1 | 71 | 0.00000 |
| 1557 | 153 | ARG | HE   | -33.79858 | -30.09360 | 110.98860 | B1 | 71 | 0.00000 |
| 1558 | 153 | ARG | CZ   | -33.01475 | -31.01372 | 109.31716 | B1 | 71 | 0.00000 |
| 1559 | 153 | ARG | NH1  | -32.97943 | -29.92906 | 108.54980 | B1 | 71 | 0.00000 |
| 1560 | 153 | ARG | NH11 | -32.81618 | -30.04802 | 107.55422 | B1 | 71 | 0.00000 |
| 1561 | 153 | ARG | NH12 | -33.14801 | -29.01024 | 108.90136 | B1 | 71 | 0.00000 |
| 1562 | 153 | ARG | NH2  | -32.57787 | -32.17691 | 108.83735 | B1 | 71 | 0.00000 |
| 1563 | 153 | ARG | NH21 | -32.40269 | -32.29042 | 107.84355 | B1 | 71 | 0.00000 |
| 1564 | 153 | ARG | NH22 | -32.45571 | -32.97359 | 109.42307 | B1 | 71 | 0.00000 |
| 1565 | 153 | ARG | C    | -37.16363 | -34.62908 | 114.06926 | B1 | 71 | 0.00000 |
| 1566 | 153 | ARG | O    | -38.37029 | -34.50228 | 113.96948 | B1 | 71 | 0.00000 |
| 1567 | 154 | ARG | N    | -36.57082 | -35.79410 | 114.34569 | B1 | 72 | 0.00000 |
| 1568 | 154 | ARG | H    | -35.57655 | -35.83805 | 114.34685 | B1 | 72 | 0.00000 |
| 1569 | 154 | ARG | CA   | -37.32441 | -37.02834 | 114.59374 | B1 | 72 | 0.00000 |
| 1570 | 154 | ARG | CB   | -36.30561 | -38.11823 | 115.12926 | B1 | 72 | 0.00000 |
| 1571 | 154 | ARG | CG   | -37.06240 | -39.46786 | 115.22908 | B1 | 72 | 0.00000 |
| 1572 | 154 | ARG | CD   | -36.14056 | -40.61269 | 115.69023 | B1 | 72 | 0.00000 |
| 1573 | 154 | ARG | NE   | -36.90866 | -41.85162 | 115.80184 | B1 | 72 | 0.00000 |
| 1574 | 154 | ARG | HE   | -37.59626 | -42.01330 | 115.09038 | B1 | 72 | 0.00000 |
| 1575 | 154 | ARG | CZ   | -36.70093 | -42.71372 | 116.80504 | B1 | 72 | 0.00000 |
| 1576 | 154 | ARG | NH1  | -37.45795 | -43.80593 | 116.88687 | B1 | 72 | 0.00000 |
| 1577 | 154 | ARG | NH11 | -37.33416 | -44.47837 | 117.61587 | B1 | 72 | 0.00000 |
| 1578 | 154 | ARG | NH12 | -38.17495 | -43.96809 | 116.20728 | B1 | 72 | 0.00000 |
| 1579 | 154 | ARG | NH2  | -35.75363 | -42.48325 | 117.71513 | B1 | 72 | 0.00000 |
| 1580 | 154 | ARG | NH21 | -35.59042 | -43.10493 | 118.48012 | B1 | 72 | 0.00000 |
| 1581 | 154 | ARG | NH22 | -35.18100 | -41.66590 | 117.63709 | B1 | 72 | 0.00000 |
| 1582 | 154 | ARG | C    | -38.52465 | -36.86141 | 115.51516 | B1 | 72 | 0.00000 |
| 1583 | 154 | ARG | O    | -39.58964 | -37.43301 | 115.28503 | B1 | 72 | 0.00000 |
| 1584 | 155 | ARG | N    | -38.35223 | -36.06670 | 116.55472 | B1 | 73 | 0.00000 |
| 1585 | 155 | ARG | H    | -37.44332 | -35.69920 | 116.77047 | B1 | 73 | 0.00000 |
| 1586 | 155 | ARG | CA   | -39.52250 | -35.72569 | 117.36371 | B1 | 73 | 0.00000 |
| 1587 | 155 | ARG | CB   | -39.05476 | -34.79593 | 118.48265 | B1 | 73 | 0.00000 |
| 1588 | 155 | ARG | CG   | -40.15723 | -34.36970 | 119.44775 | B1 | 73 | 0.00000 |
| 1589 | 155 | ARG | CD   | -39.62900 | -33.36327 | 120.46128 | B1 | 73 | 0.00000 |
| 1590 | 155 | ARG | NE   | -40.71623 | -32.83780 | 121.28237 | B1 | 73 | 0.00000 |
| 1591 | 155 | ARG | HE   | -41.63763 | -33.18145 | 121.09517 | B1 | 73 | 0.00000 |
| 1592 | 155 | ARG | CZ   | -40.47089 | -31.92135 | 122.22743 | B1 | 73 | 0.00000 |
| 1593 | 155 | ARG | NH1  | -41.46382 | -31.43599 | 122.94081 | B1 | 73 | 0.00000 |
| 1594 | 155 | ARG | NH11 | -41.33886 | -30.75247 | 123.65592 | B1 | 73 | 0.00000 |
| 1595 | 155 | ARG | NH12 | -42.41818 | -31.75018 | 122.77039 | B1 | 73 | 0.00000 |
| 1596 | 155 | ARG | NH2  | -39.22715 | -31.49669 | 122.45304 | B1 | 73 | 0.00000 |

FIG. 26

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|      |         |      |           |           |           |    |    |         |
|------|---------|------|-----------|-----------|-----------|----|----|---------|
| 1597 | 155 AR  | HH21 | -39.02013 | -30.81248 | 123.15141 | B1 | 73 | 0.00000 |
| 1598 | 155 ARG | HH22 | -38.47020 | -31.56739 | 121.91409 | B1 | 73 | 0.00000 |
| 1599 | 155 ARG | C    | -40.65389 | -35.07891 | 116.56312 | B1 | 73 | 0.00000 |
| 1600 | 155 ARG | O    | -41.80290 | -35.51173 | 116.56408 | B1 | 73 | 0.00000 |
| 1601 | 155 ALA | N    | -40.28792 | -34.01372 | 115.84199 | B1 | 74 | 0.00000 |
| 1602 | 155 ALA | H    | -39.31961 | -33.75543 | 115.77185 | B1 | 74 | 0.00000 |
| 1603 | 155 ALA | CA   | -41.30773 | -33.34228 | 115.03220 | B1 | 74 | 0.00000 |
| 1604 | 155 ALA | CB   | -40.72599 | -32.10051 | 114.35248 | B1 | 74 | 0.00000 |
| 1605 | 155 ALA | C    | -41.91382 | -34.25984 | 113.98113 | B1 | 74 | 0.00000 |
| 1606 | 155 ALA | O    | -43.11961 | -34.40803 | 113.53911 | B1 | 74 | 0.00000 |
| 1607 | 157 VAL | N    | -40.99693 | -34.92630 | 113.26026 | B1 | 75 | 0.00000 |
| 1608 | 157 VAL | H    | -40.04150 | -34.58533 | 113.44509 | B1 | 75 | 0.00000 |
| 1609 | 157 VAL | CA   | -41.27013 | -35.00533 | 112.34552 | B1 | 75 | 0.00000 |
| 1610 | 157 VAL | CB   | -39.85551 | -35.59597 | 112.04095 | B1 | 75 | 0.00000 |
| 1611 | 157 VAL | CG1  | -39.79482 | -35.01333 | 111.48596 | B1 | 75 | 0.00000 |
| 1612 | 157 VAL | CG2  | -39.10167 | -35.63993 | 111.12688 | B1 | 75 | 0.00000 |
| 1613 | 157 VAL | C    | -42.31375 | -37.01997 | 112.83333 | B1 | 75 | 0.00000 |
| 1614 | 157 VAL | O    | -43.41555 | -37.10248 | 112.30297 | B1 | 75 | 0.00000 |
| 1615 | 158 ASP | N    | -41.95045 | -37.78157 | 113.87061 | B1 | 75 | 0.00000 |
| 1616 | 158 ASP | H    | -41.05305 | -37.58874 | 114.30470 | B1 | 75 | 0.00000 |
| 1617 | 158 ASP | CA   | -43.55516 | -38.84272 | 114.32359 | B1 | 75 | 0.00000 |
| 1618 | 158 ASP | CB   | -42.09373 | -39.82201 | 115.22733 | B1 | 75 | 0.00000 |
| 1619 | 158 ASP | CG   | -41.27306 | -40.78302 | 114.39952 | B1 | 75 | 0.00000 |
| 1620 | 158 ASP | OD1  | -40.34839 | -40.37834 | 113.70459 | B1 | 75 | 0.00000 |
| 1621 | 158 ASP | OD2  | -41.56822 | -41.98359 | 114.41807 | B1 | 75 | 0.00000 |
| 1622 | 158 ASP | C    | -44.10543 | -38.36705 | 115.04358 | B1 | 75 | 0.00000 |
| 1623 | 158 ASP | O    | -45.17033 | -38.96720 | 114.93521 | B1 | 75 | 0.00000 |
| 1624 | 159 THR | N    | -43.95505 | -37.25912 | 115.79951 | B1 | 77 | 0.00000 |
| 1625 | 159 THR | H    | -43.09027 | -35.75113 | 115.56564 | B1 | 77 | 0.00000 |
| 1626 | 159 THR | CA   | -45.15504 | -36.89791 | 116.55067 | B1 | 77 | 0.00000 |
| 1627 | 159 THR | CB   | -44.86388 | -36.97162 | 116.07412 | B1 | 77 | 0.00000 |
| 1628 | 159 THR | CG1  | -45.06916 | -37.10329 | 116.79712 | B1 | 77 | 0.00000 |
| 1629 | 159 THR | CG2  | -45.91547 | -37.30091 | 119.72205 | B1 | 77 | 0.00000 |
| 1630 | 159 THR | C    | -44.03422 | -35.82524 | 115.66004 | B1 | 77 | 0.00000 |
| 1631 | 159 THR | O    | -45.84489 | -35.59150 | 116.12087 | B1 | 77 | 0.00000 |
| 1632 | 159 THR | N    | -47.05165 | -35.51845 | 115.96755 | B1 | 77 | 0.00000 |
| 1633 | 160 TYR | N    | -45.05289 | -34.84372 | 115.87045 | B1 | 78 | 0.00000 |
| 1634 | 160 TYR | H    | -44.05561 | -34.64495 | 115.78833 | B1 | 78 | 0.00000 |
| 1635 | 160 TYR | CA   | -45.73493 | -33.26591 | 115.64281 | B1 | 78 | 0.00000 |
| 1636 | 160 TYR | CB   | -44.74473 | -32.10745 | 115.78675 | B1 | 78 | 0.00000 |
| 1637 | 160 TYR | CG   | -45.25402 | -31.12355 | 116.81319 | B1 | 78 | 0.00000 |
| 1638 | 160 TYR | CD1  | -44.55214 | -31.25590 | 116.16144 | B1 | 78 | 0.00000 |
| 1639 | 160 TYR | CE1  | -45.32919 | -30.34310 | 119.12525 | B1 | 78 | 0.00000 |
| 1640 | 160 TYR | CD2  | -45.12744 | -30.08443 | 116.42011 | B1 | 78 | 0.00000 |
| 1641 | 160 TYR | CE2  | -46.50347 | -29.17117 | 117.38455 | B1 | 78 | 0.00000 |
| 1642 | 160 TYR | CZ   | -45.20180 | -29.30409 | 115.73381 | B1 | 78 | 0.00000 |
| 1643 | 160 TYR | OH   | -45.55272 | -28.41253 | 119.68223 | B1 | 78 | 0.00000 |
| 1644 | 160 TYR | HH   | -47.25242 | -27.80044 | 119.27249 | B1 | 78 | 0.00000 |
| 1645 | 160 TYR | C    | -45.45009 | -33.18254 | 114.31073 | B1 | 78 | 0.00000 |
| 1646 | 160 TYR | O    | -47.53057 | -32.82958 | 114.21477 | B1 | 78 | 0.00000 |
| 1647 | 161 CYS | N    | -45.72598 | -33.55992 | 113.36774 | B1 | 79 | 0.00000 |
| 1648 | 161 CYS | H    | -44.77052 | -33.58209 | 113.40718 | B1 | 79 | 0.00000 |
| 1649 | 161 CYS | CA   | -46.32703 | -33.65577 | 111.93544 | B1 | 79 | 0.00000 |
| 1650 | 161 CYS | CB   | -45.27134 | -34.17403 | 110.93055 | B1 | 79 | 0.00000 |
| 1651 | 161 CYS | CG   | -46.67069 | -33.53715 | 109.19024 | B1 | 79 | 0.00000 |
| 1652 | 161 CYS | C    | -47.53731 | -34.50219 | 111.93084 | B1 | 79 | 0.00000 |
| 1653 | 161 CYS | O    | -45.55723 | -34.29704 | 111.38273 | B1 | 79 | 0.00000 |
| 1654 | 162 ARG | N    | -47.37452 | -35.72005 | 112.55592 | B1 | 80 | 0.00000 |
| 1655 | 162 ARG | H    | -45.47835 | -35.94232 | 113.03852 | B1 | 80 | 0.00000 |
| 1656 | 162 ARG | CA   | -45.50575 | -35.51754 | 112.89065 | B1 | 80 | 0.00000 |
| 1657 | 162 ARG | CB   | -45.07710 | -37.71515 | 113.55475 | B1 | 80 | 0.00000 |
| 1658 | 162 ARG | CG   | -45.16345 | -38.77197 | 114.12227 | B1 | 80 | 0.00000 |
| 1659 | 162 ARG | CD   | -45.67544 | -40.04247 | 114.81523 | B1 | 80 | 0.00000 |
| 1660 | 162 ARG | NE   | -49.62321 | -41.12379 | 114.54199 | B1 | 80 | 0.00000 |

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|      |     |     |      |           |           |           |    |    |         |
|------|-----|-----|------|-----------|-----------|-----------|----|----|---------|
| 1661 | 162 | ARG | HE   | -50.94    | -40.88455 | 114.11092 | B1 | 80 | 0.00000 |
| 1662 | 162 | ARG | CZ   | -49.3267  | -42.40507 | 114.80601 | B1 | 80 | 0.00000 |
| 1663 | 162 | ARG | NH1  | -50.23020 | -43.32564 | 114.46730 | B1 | 80 | 0.00000 |
| 1664 | 162 | ARG | NH11 | -50.11979 | -44.31403 | 114.66150 | B1 | 80 | 0.00000 |
| 1665 | 162 | ARG | NH12 | -51.06184 | -43.06285 | 113.96028 | B1 | 80 | 0.00000 |
| 1666 | 162 | ARG | NH2  | -48.19839 | -42.76163 | 115.38323 | B1 | 80 | 0.00000 |
| 1667 | 162 | ARG | NH21 | -48.00134 | -43.72771 | 115.55650 | B1 | 80 | 0.00000 |
| 1668 | 162 | ARG | NH22 | -47.52579 | -42.06788 | 115.64161 | B1 | 80 | 0.00000 |
| 1669 | 162 | ARG | C    | -49.75512 | -35.92906 | 113.42487 | B1 | 80 | 0.00000 |
| 1670 | 162 | ARG | O    | -50.82093 | -35.93732 | 112.81658 | B1 | 80 | 0.00000 |
| 1671 | 163 | HIS | N    | -49.58593 | -35.31862 | 114.60088 | B1 | 81 | 0.00000 |
| 1672 | 163 | HIS | H    | -48.68252 | -35.28035 | 115.03933 | B1 | 81 | 0.00000 |
| 1673 | 163 | HIS | CA   | -50.76431 | -34.73357 | 115.23467 | B1 | 81 | 0.00000 |
| 1674 | 163 | HIS | CB   | -50.42874 | -34.29045 | 116.66134 | B1 | 81 | 0.00000 |
| 1675 | 163 | HIS | CG   | -50.41026 | -35.50649 | 117.55950 | B1 | 81 | 0.00000 |
| 1676 | 163 | HIS | ND1  | -51.51644 | -36.01842 | 118.12240 | B1 | 81 | 0.00000 |
| 1677 | 163 | HIS | HD1  | -52.42830 | -35.67431 | 118.03242 | B1 | 81 | 0.00000 |
| 1678 | 163 | HIS | CD2  | -49.31404 | -36.28837 | 117.93420 | B1 | 81 | 0.00000 |
| 1679 | 163 | HIS | NE2  | -49.78030 | -37.28089 | 118.73130 | B1 | 81 | 0.00000 |
| 1680 | 163 | HIS | CE1  | -51.13423 | -37.11585 | 118.84798 | B1 | 81 | 0.00000 |
| 1681 | 163 | HIS | C    | -51.37160 | -33.59588 | 114.44466 | B1 | 81 | 0.00000 |
| 1682 | 163 | HIS | O    | -52.56947 | -33.55956 | 114.18659 | B1 | 81 | 0.00000 |
| 1683 | 164 | ASN | N    | -50.50246 | -32.67616 | 114.01202 | B1 | 82 | 0.00000 |
| 1684 | 164 | ASN | H    | -49.51981 | -32.74462 | 114.21247 | B1 | 82 | 0.00000 |
| 1685 | 164 | ASN | CA   | -51.04300 | -31.58239 | 113.20331 | B1 | 82 | 0.00000 |
| 1686 | 164 | ASN | CB   | -49.96583 | -30.54361 | 112.89196 | B1 | 82 | 0.00000 |
| 1687 | 164 | ASN | CG   | -49.91907 | -29.53869 | 114.02377 | B1 | 82 | 0.00000 |
| 1688 | 164 | ASN | OD1  | -49.13948 | -29.62233 | 114.96163 | B1 | 82 | 0.00000 |
| 1689 | 164 | ASN | ND2  | -50.80473 | -28.55321 | 113.91309 | B1 | 82 | 0.00000 |
| 1690 | 164 | ASN | HD21 | -51.44311 | -28.49843 | 113.14586 | B1 | 82 | 0.00000 |
| 1691 | 164 | ASN | HD22 | -50.84210 | -27.84178 | 114.61251 | B1 | 82 | 0.00000 |
| 1692 | 164 | ASN | C    | -51.70674 | -32.02333 | 111.91584 | B1 | 82 | 0.00000 |
| 1693 | 164 | ASN | O    | -52.73418 | -31.48662 | 111.51085 | B1 | 82 | 0.00000 |
| 1694 | 165 | TYR | N    | -51.12326 | -33.05626 | 111.29191 | B1 | 83 | 0.00000 |
| 1695 | 165 | TYR | H    | -50.28201 | -33.49370 | 111.62194 | B1 | 83 | 0.00000 |
| 1696 | 165 | TYR | CA   | -51.81304 | -33.54151 | 110.10401 | B1 | 83 | 0.00000 |
| 1697 | 165 | TYR | CB   | -50.52781 | -34.47239 | 109.25048 | B1 | 83 | 0.00000 |
| 1698 | 165 | TYR | CG   | -51.39689 | -34.50284 | 107.80317 | B1 | 83 | 0.00000 |
| 1699 | 165 | TYR | CD1  | -52.18946 | -33.44669 | 107.29137 | B1 | 83 | 0.00000 |
| 1700 | 165 | TYR | CE1  | -52.63312 | -33.47413 | 105.96126 | B1 | 83 | 0.00000 |
| 1701 | 165 | TYR | CD2  | -51.04289 | -35.58963 | 106.96903 | B1 | 83 | 0.00000 |
| 1702 | 165 | TYR | CE2  | -51.48846 | -35.61522 | 105.62740 | B1 | 83 | 0.00000 |
| 1703 | 165 | TYR | CZ   | -52.28557 | -34.55457 | 105.13440 | B1 | 83 | 0.00000 |
| 1704 | 165 | TYR | OH   | -52.75931 | -34.53152 | 103.84155 | B1 | 83 | 0.00000 |
| 1705 | 165 | TYR | NH   | -52.13515 | -34.97162 | 103.24416 | B1 | 83 | 0.00000 |
| 1706 | 165 | TYR | C    | -53.16114 | -34.17050 | 110.39688 | B1 | 83 | 0.00000 |
| 1707 | 165 | TYR | O    | -54.17243 | -33.75040 | 109.85354 | B1 | 83 | 0.00000 |
| 1708 | 166 | GLY | N    | -53.16827 | -35.13255 | 111.32677 | B1 | 84 | 0.00000 |
| 1709 | 166 | GLY | H    | -52.30920 | -35.44284 | 111.74443 | B1 | 84 | 0.00000 |
| 1710 | 166 | GLY | CA   | -54.44388 | -35.75931 | 111.69489 | B1 | 84 | 0.00000 |
| 1711 | 166 | GLY | C    | -55.55421 | -34.78683 | 112.08191 | B1 | 84 | 0.00000 |
| 1712 | 166 | GLY | O    | -56.70058 | -34.86763 | 111.64884 | B1 | 84 | 0.00000 |
| 1713 | 167 | VAL | N    | -55.16433 | -33.81049 | 112.90998 | B1 | 85 | 0.00000 |
| 1714 | 167 | VAL | H    | -54.21931 | -33.77699 | 113.25020 | B1 | 85 | 0.00000 |
| 1715 | 167 | VAL | CA   | -56.14083 | -32.77588 | 113.26808 | B1 | 85 | 0.00000 |
| 1716 | 167 | VAL | CB   | -55.54422 | -31.87200 | 114.36486 | B1 | 85 | 0.00000 |
| 1717 | 167 | VAL | CG1  | -56.46931 | -30.71890 | 114.75691 | B1 | 85 | 0.00000 |
| 1718 | 167 | VAL | CG2  | -55.22649 | -32.70528 | 115.60849 | B1 | 85 | 0.00000 |
| 1719 | 167 | VAL | C    | -56.62003 | -31.96437 | 112.06515 | B1 | 85 | 0.00000 |
| 1720 | 167 | VAL | O    | -57.80658 | -31.70971 | 111.87315 | B1 | 85 | 0.00000 |
| 1721 | 168 | GLY | N    | -55.65605 | -31.61592 | 111.20320 | B1 | 86 | 0.00000 |
| 1722 | 168 | GLY | H    | -54.68827 | -31.81924 | 111.38362 | B1 | 86 | 0.00000 |
| 1723 | 168 | GLY | CA   | -56.04215 | -30.94490 | 109.94972 | B1 | 86 | 0.00000 |
| 1724 | 168 | GLY | C    | -57.02338 | -31.77629 | 109.11567 | B1 | 86 | 0.00000 |

FIG. 28

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|      |     |     |        |           |           |           |    |         |         |
|------|-----|-----|--------|-----------|-----------|-----------|----|---------|---------|
| 1725 | 168 | GLY | -58.49 | -31.28044 | 108.61617 | B1        | 86 | 0.00000 |         |
| 1726 | 169 | GLU | N      | -56.71134 | -33.07169 | 109.00665 | B1 | 87      | 0.00000 |
| 1727 | 169 | GLU | H      | -55.87921 | -33.43085 | 109.43169 | B1 | 87      | 0.00000 |
| 1728 | 169 | GLU | CA     | -57.59179 | -34.00467 | 108.30469 | B1 | 87      | 0.00000 |
| 1729 | 169 | GLU | CB     | -56.95070 | -35.39155 | 108.28846 | B1 | 87      | 0.00000 |
| 1730 | 169 | GLU | CG     | -55.67851 | -35.40281 | 107.43481 | B1 | 87      | 0.00000 |
| 1731 | 169 | GLU | CD     | -54.91259 | -36.69049 | 107.65905 | B1 | 87      | 0.00000 |
| 1732 | 169 | GLU | OE1    | -53.74095 | -36.61342 | 108.02205 | B1 | 87      | 0.00000 |
| 1733 | 169 | GLU | OE2    | -55.48540 | -37.76250 | 107.47736 | B1 | 87      | 0.00000 |
| 1734 | 169 | GLU | C      | -59.00151 | -34.05273 | 108.86565 | B1 | 87      | 0.00000 |
| 1735 | 169 | GLU | O      | -59.98966 | -34.06690 | 108.14126 | B1 | 87      | 0.00000 |
| 1736 | 170 | SER | N      | -59.06996 | -33.99305 | 110.19884 | B1 | 88      | 0.00000 |
| 1737 | 170 | SER | H      | -50.23138 | -34.05998 | 110.74831 | B1 | 88      | 0.00000 |
| 1738 | 170 | SER | CA     | -60.38255 | -33.85094 | 110.83391 | B1 | 88      | 0.00000 |
| 1739 | 170 | SER | CB     | -60.18950 | -33.85581 | 112.35798 | B1 | 88      | 0.00000 |
| 1740 | 170 | SER | OG     | -61.42043 | -34.13237 | 113.03659 | B1 | 88      | 0.00000 |
| 1741 | 170 | SER | HG     | -61.30877 | -34.00943 | 113.98374 | B1 | 88      | 0.00000 |
| 1742 | 170 | SER | C      | -61.16415 | -32.61665 | 110.37646 | B1 | 88      | 0.00000 |
| 1743 | 170 | SER | O      | -62.31497 | -32.69150 | 109.96191 | B1 | 88      | 0.00000 |
| 1744 | 171 | PHE | N      | -60.49231 | -31.45621 | 110.41676 | B1 | 89      | 0.00000 |
| 1745 | 171 | PHE | H      | -59.54601 | -31.41832 | 110.75393 | B1 | 89      | 0.00000 |
| 1746 | 171 | PHE | CA     | -61.19539 | -30.24631 | 109.95663 | B1 | 89      | 0.00000 |
| 1747 | 171 | PHE | CB     | -60.30793 | -28.99941 | 110.10880 | B1 | 89      | 0.00000 |
| 1748 | 171 | PHE | CG     | -59.94208 | -28.68147 | 111.54294 | B1 | 89      | 0.00000 |
| 1749 | 171 | PHE | CD1    | -58.59291 | -20.39703 | 111.85413 | B1 | 89      | 0.00000 |
| 1750 | 171 | PHE | CD2    | -60.93098 | -20.63398 | 112.55491 | B1 | 89      | 0.00000 |
| 1751 | 171 | PHE | CE1    | -58.23032 | -28.06074 | 113.17656 | B1 | 89      | 0.00000 |
| 1752 | 171 | PHE | CE2    | -60.56845 | -28.29967 | 113.87858 | B1 | 89      | 0.00000 |
| 1753 | 171 | PHE | CZ     | -59.21901 | -28.01319 | 114.18527 | B1 | 89      | 0.00000 |
| 1754 | 171 | PHE | C      | -61.62802 | -30.29139 | 108.49502 | B1 | 89      | 0.00000 |
| 1755 | 171 | PHE | O      | -62.68697 | -29.84047 | 108.07691 | B1 | 89      | 0.00000 |
| 1756 | 172 | THR | N      | -60.72520 | -30.85206 | 107.69903 | B1 | 90      | 0.00000 |
| 1757 | 172 | THR | H      | -59.91792 | -31.29854 | 108.09636 | B1 | 90      | 0.00000 |
| 1758 | 172 | THR | CA     | -60.04308 | -30.66246 | 106.25599 | B1 | 90      | 0.00000 |
| 1759 | 172 | THR | CB     | -59.41710 | -30.70747 | 105.70165 | B1 | 90      | 0.00000 |
| 1760 | 172 | THR | OG1    | -59.35292 | -30.21143 | 104.36207 | B1 | 90      | 0.00000 |
| 1761 | 172 | THR | HG1    | -60.15430 | -30.48800 | 103.89285 | B1 | 90      | 0.00000 |
| 1762 | 172 | THR | CG2    | -58.90262 | -32.13906 | 105.74825 | B1 | 90      | 0.00000 |
| 1763 | 172 | THR | C      | -61.71208 | -31.64677 | 105.47987 | B1 | 90      | 0.00000 |
| 1764 | 172 | THR | O      | -61.76078 | -31.56505 | 104.25169 | B1 | 90      | 0.00000 |
| 1765 | 173 | VAL | N      | -62.32957 | -32.60764 | 106.19315 | B1 | 91      | 0.00000 |
| 1766 | 173 | VAL | H      | -62.28706 | -32.56397 | 107.19363 | B1 | 91      | 0.00000 |
| 1767 | 173 | VAL | CA     | -62.87984 | -33.81113 | 105.53718 | B1 | 91      | 0.00000 |
| 1768 | 173 | VAL | CB     | -63.87967 | -34.51911 | 106.47899 | B1 | 91      | 0.00000 |
| 1769 | 173 | VAL | CG1    | -64.50006 | -35.77324 | 105.85034 | B1 | 91      | 0.00000 |
| 1770 | 173 | VAL | CG2    | -63.20452 | -34.90248 | 107.79466 | B1 | 91      | 0.00000 |
| 1771 | 173 | VAL | C      | -63.51710 | -33.59419 | 104.16716 | B1 | 91      | 0.00000 |
| 1772 | 173 | VAL | O      | -63.18750 | -34.24452 | 103.18126 | B1 | 91      | 0.00000 |
| 1773 | 174 | GLN | N      | -64.41211 | -32.59570 | 104.14711 | B1 | 92      | 0.00000 |
| 1774 | 174 | GLN | H      | -64.59818 | -32.11269 | 105.00138 | B1 | 92      | 0.00000 |
| 1775 | 174 | GLN | CA     | -65.14373 | -32.19104 | 102.94243 | B1 | 92      | 0.00000 |
| 1776 | 174 | GLN | CB     | -65.76132 | -30.80951 | 103.22574 | B1 | 92      | 0.00000 |
| 1777 | 174 | GLN | CG     | -66.77986 | -30.26016 | 102.21318 | B1 | 92      | 0.00000 |
| 1778 | 174 | GLN | CD     | -66.09397 | -29.58024 | 101.04012 | B1 | 92      | 0.00000 |
| 1779 | 174 | GLN | OE1    | -65.45924 | -20.54065 | 101.15380 | B1 | 92      | 0.00000 |
| 1780 | 174 | GLN | NE2    | -66.26402 | -30.18961 | 99.87453  | B1 | 92      | 0.00000 |
| 1781 | 174 | GLN | HE21   | -66.63226 | -31.11966 | 99.82928  | B1 | 92      | 0.00000 |
| 1782 | 174 | GLN | HE22   | -65.97833 | -29.74839 | 99.02730  | B1 | 92      | 0.00000 |
| 1783 | 174 | GLN | C      | -64.36067 | -32.16074 | 101.63553 | B1 | 92      | 0.00000 |
| 1784 | 174 | GLN | O      | -64.88582 | -32.51356 | 100.57991 | B1 | 92      | 0.00000 |
| 1785 | 175 | ARG | N      | -63.09233 | -31.77447 | 101.73327 | B1 | 93      | 0.00000 |
| 1786 | 175 | ARG | H      | -62.69754 | -31.53564 | 102.62225 | B1 | 93      | 0.00000 |
| 1787 | 175 | ARG | CA     | -62.31707 | -31.78635 | 100.50018 | B1 | 93      | 0.00000 |
| 1788 | 175 | ARG | CB     | -61.85817 | -30.36631 | 100.16958 | B1 | 93      | 0.00000 |

FIG. 29

00013077 012698

09013077.012698

..DR1\_MIN2.CRD

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29

|      |     |     |      |           |           |           |    |    |          |
|------|-----|-----|------|-----------|-----------|-----------|----|----|----------|
| 1789 | 175 | ARG | CG   | -61.24395 | -30.26914 | 98.77310  | B1 | 93 | 0.000000 |
| 1790 | 175 | ARG | CD   | -60.91597 | -28.04209 | 98.34709  | B1 | 93 | 0.000000 |
| 1791 | 175 | ARG | NE   | -59.98117 | -28.87216 | 97.22615  | B1 | 93 | 0.000000 |
| 1792 | 175 | ARG | HE   | -59.59146 | -29.76910 | 97.00518  | B1 | 93 | 0.000000 |
| 1793 | 175 | ARG | CZ   | -59.49795 | -27.74924 | 96.68186  | B1 | 93 | 0.000000 |
| 1794 | 175 | ARG | NH1  | -58.57343 | -27.83579 | 95.72833  | B1 | 93 | 0.000000 |
| 1795 | 175 | ARG | HH11 | -58.19414 | -27.02728 | 95.28229  | B1 | 93 | 0.000000 |
| 1796 | 175 | ARG | HH12 | -58.22480 | -28.73459 | 95.46034  | B1 | 93 | 0.000000 |
| 1797 | 175 | ARG | NH2  | -59.92427 | -26.55682 | 97.09593  | B1 | 93 | 0.000000 |
| 1798 | 175 | ARG | HH21 | -59.57028 | -25.70796 | 96.70808  | B1 | 93 | 0.000000 |
| 1799 | 175 | ARG | HH22 | -60.60311 | -26.50975 | 97.82696  | B1 | 93 | 0.000000 |
| 1800 | 175 | ARG | C    | -61.17336 | -32.79150 | 100.46150 | B1 | 93 | 0.000000 |
| 1801 | 175 | ARG | O    | -61.02327 | -33.52738 | 99.49809  | B1 | 93 | 0.000000 |
| 1802 | 176 | ARG | N    | -60.36493 | -32.85103 | 101.53216 | B1 | 94 | 0.000000 |
| 1803 | 176 | ARG | H    | -60.53761 | -32.31340 | 102.35642 | B1 | 94 | 0.000000 |
| 1804 | 176 | ARG | CA   | -59.25084 | -33.80802 | 101.41499 | B1 | 94 | 0.000000 |
| 1805 | 176 | ARG | CB   | -58.18750 | -33.62483 | 102.49829 | B1 | 94 | 0.000000 |
| 1806 | 176 | ARG | CG   | -57.32871 | -32.37173 | 102.34974 | B1 | 94 | 0.000000 |
| 1807 | 176 | ARG | CD   | -56.27515 | -32.28237 | 103.45854 | B1 | 94 | 0.000000 |
| 1808 | 176 | ARG | NE   | -56.30062 | -30.94018 | 104.04511 | B1 | 94 | 0.000000 |
| 1809 | 176 | ARG | HE   | -56.83150 | -30.25818 | 103.53710 | B1 | 94 | 0.000000 |
| 1810 | 176 | ARG | CZ   | -55.69078 | -30.63659 | 105.15759 | B1 | 94 | 0.000000 |
| 1811 | 176 | ARG | NH1  | -55.74431 | -29.38340 | 105.64628 | B1 | 94 | 0.000000 |
| 1812 | 176 | ARG | HH11 | -55.30471 | -29.10555 | 106.50132 | B1 | 94 | 0.000000 |
| 1813 | 176 | ARG | HH12 | -56.24080 | -28.69008 | 105.12278 | B1 | 94 | 0.000000 |
| 1814 | 176 | ARG | NH2  | -55.05038 | -31.57276 | 105.85297 | B1 | 94 | 0.000000 |
| 1815 | 176 | ARG | HH21 | -54.58912 | -31.37726 | 106.75753 | B1 | 94 | 0.000000 |
| 1816 | 176 | ARG | HH22 | -55.02183 | -32.51329 | 105.54660 | B1 | 94 | 0.000000 |
| 1817 | 176 | ARG | C    | -59.64666 | -35.27348 | 101.42902 | B1 | 94 | 0.000000 |
| 1818 | 176 | ARG | O    | -58.87808 | -36.15316 | 101.06767 | B1 | 94 | 0.000000 |
| 1819 | 177 | VAL | N    | -60.88626 | -35.53390 | 101.85272 | B1 | 95 | 0.000000 |
| 1820 | 177 | VAL | H    | -61.51901 | -34.82991 | 102.18430 | B1 | 95 | 0.000000 |
| 1821 | 177 | VAL | CA   | -61.32863 | -36.91608 | 101.70299 | B1 | 95 | 0.000000 |
| 1822 | 177 | VAL | CB   | -61.79519 | -37.47193 | 103.06780 | B1 | 95 | 0.000000 |
| 1823 | 177 | VAL | CG1  | -61.84113 | -39.00335 | 103.05589 | B1 | 95 | 0.000000 |
| 1824 | 177 | VAL | CG2  | -60.88761 | -37.00753 | 104.21299 | B1 | 95 | 0.000000 |
| 1825 | 177 | VAL | C    | -62.41412 | -37.02458 | 100.63553 | B1 | 95 | 0.000000 |
| 1826 | 177 | VAL | O    | -63.44404 | -37.67295 | 100.79118 | B1 | 95 | 0.000000 |
| 1827 | 178 | HIS | N    | -62.14889 | -36.33028 | 99.52296  | B1 | 96 | 0.000000 |
| 1828 | 178 | HIS | H    | -61.32158 | -35.77698 | 99.39184  | B1 | 96 | 0.000000 |
| 1829 | 178 | HIS | CA   | -63.09845 | -36.32813 | 98.41659  | B1 | 96 | 0.000000 |
| 1830 | 178 | HIS | CB   | -64.01495 | -35.10064 | 98.57314  | B1 | 96 | 0.000000 |
| 1831 | 178 | HIS | CG   | -65.27852 | -35.21481 | 97.74669  | B1 | 96 | 0.000000 |
| 1832 | 178 | HIS | ND1  | -65.30573 | -35.62002 | 96.46944  | B1 | 96 | 0.000000 |
| 1833 | 178 | HIS | HD1  | -64.50806 | -35.91855 | 95.96816  | B1 | 96 | 0.000000 |
| 1834 | 178 | HIS | CD2  | -66.58524 | -34.92566 | 98.14872  | B1 | 96 | 0.000000 |
| 1835 | 178 | HIS | NE2  | -67.39749 | -35.16505 | 97.08780  | B1 | 96 | 0.000000 |
| 1836 | 178 | HIS | CE1  | -66.60728 | -35.59364 | 96.05191  | B1 | 96 | 0.000000 |
| 1837 | 178 | HIS | C    | -62.34621 | -36.29235 | 97.09131  | B1 | 96 | 0.000000 |
| 1838 | 178 | HIS | OCT1 | -61.22615 | -35.78756 | 97.07091  | B1 | 96 | 0.000000 |
| 1839 | 178 | HIS | OCT2 | -62.87363 | -36.77415 | 96.08799  | B1 | 96 | 0.000000 |

FIG. 30

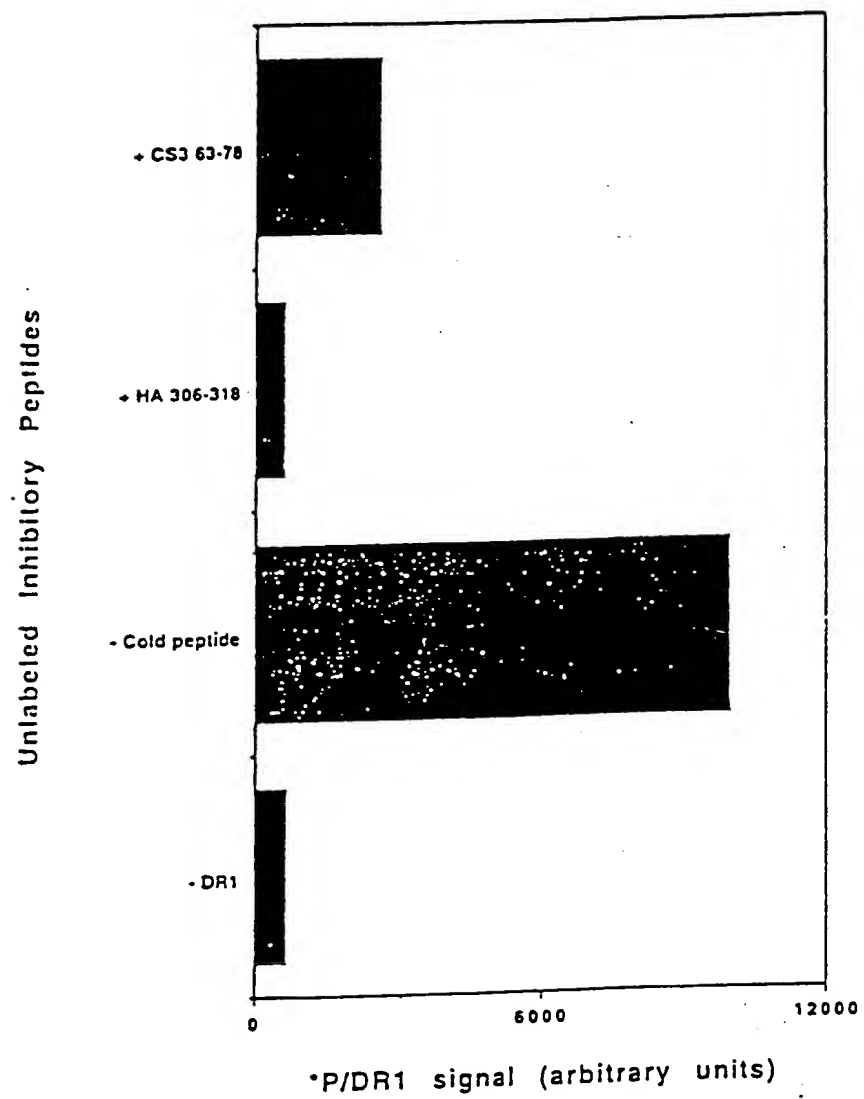
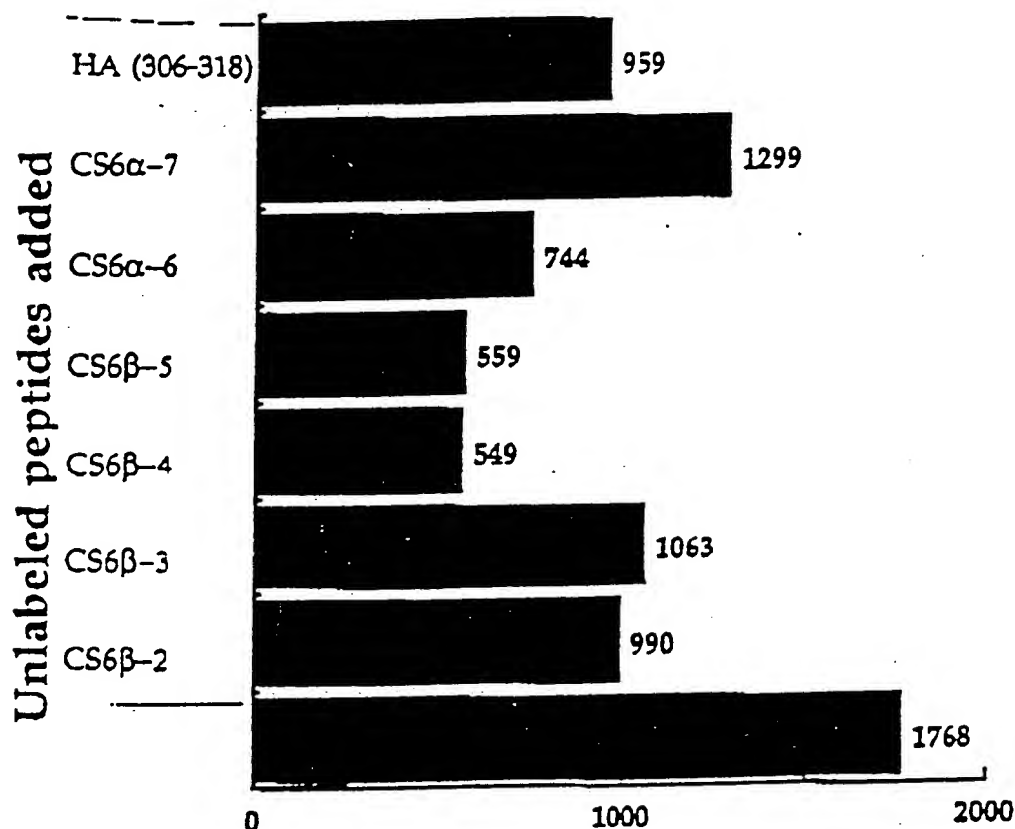


FIG. 31

# Inhibition of $^{125}\text{I}$ HA(306-318)/DR1 by unlabeled CS6 $\alpha$ and $\beta$ peptides



\*HA/DR1 compact dimer signal  
(densitometric units)